Air Quality Modeling

Appendix C

Introduction

Section 812 of the 1990 Clean Air Act Amendments (CAAA) requires the U.S. Environmental Protection Agency (EPA) to perform periodic, comprehensive, prospective analyses of the costs and benefits associated with programs implemented pursuant to the Clean Air Act (CAA). Such analysis requires the estimation of future-year emissions levels and associated air-quality-related values for scenarios reflecting compliance with the CAA, as well as for scenarios for which the effects of programs associated with the CAA are not accounted for in establishing the future-year estimates. This report summarizes the results of an air quality modeling and analysis study designed to estimate the effects of the CAAA on future air quality. The Section 812 prospective study includes analysis of following criteria pollutants: ozone, particulate matter (PM), sulfur dioxide (SO_2), nitrogen oxide (NO), nitrogen dioxide (NO_2), and carbon monoxide (CO). Future-year estimates of these atmospheric constituents were obtained through the application of air quality modeling tools and techniques, as described in this report.

An integral component of the modeling analysis was the estimation of future-year emission levels associated with the two CAAA scenarios and two future years. Scenarios that incorporate the emission reductions associated with CAAA are referred to as Post-CAAA while those that incorporate growth but reflect 1990 regulations are referred to as Pre-CAAA. The two future years considered in the analysis are 2000 and 2010. The emissions estimates (Pechan, 1998) provide the basis for the estimation of ozone, PM, and other criteria pollutant concentrations associated with each scenario and future year.

Future-year estimates of ozone concentrations were obtained through the combined application of the Urban Airshed Model (UAM) and the variable-grid UAM (UAM-V), yielding urban- and/or regional-scale estimates of ozone concentrations for each scenario and future year for the entire U.S. (48 contiguous states).

Concentrations of primary and secondary PM for the future-year scenarios (including PM_{10}, with a diameter of less than 10 micrometers, and $PM_{2.5}$, with a diameter of less than 2.5 micrometers) were estimated through the combined application of the Regional Acid Deposition Model/Regional Particulate Model (RADM/RPM) and the Regulatory Modeling System for Aerosols and Acid Deposition (REMSAD). RADM/RPM was used for the eastern U.S., while REMSAD was applied to the analysis of PM within the western U.S.

An emissions-based, linear "roll-back" technique was used to estimate future-year concentrations for the other pollutants considered as part of this analysis – SO_2, NO, NO_2, and CO.

Following application of the modeling techniques, site-specific estimates of future-year air quality were obtained by adjusting observational data (corresponding to a base year of 1990) in accordance with the changes in air quality predicted by the modeling systems. Statistical quantities or "profiles" describing the predicted concentration distributions for each monitoring site were then calculated. The resulting statistical concentration distributions provide the basis for the examination and quantification of the effects of changes in air quality on health, agriculture, and the economy (i.e., physical effects and economic valuation modeling) resulting from compliance with the CAAA.

The remainder of this report summarizes the methods and results of the section 812 prospective air quality modeling analysis. An overview of the modeling/analysis methodology is provided in section 2. The methods and results for ozone are presented in section 3. The methods and results for PM are

provided in section 4. The linear-rollback modeling for the other criteria pollutants is summarized in section 5. A discussion of the attributes and limitations of the modeling analysis methodologies is provided in section 6. Finally, recommendations for further research are given in section 7.

Overview of the Section 812 Prospective Modeling Analysis

The air quality modeling component of the section 812 prospective analysis included the application of a variety of air quality modeling tools and techniques, as well as the combined use of observational data and modeling results to estimate future-year concentrations of several criteria pollutants. An overview of the modeling approach is provided in this section of the report.

The overall objective of the modeling exercise was to provide base- and future-year estimates of ozone, PM, SO_2, NO, NO_2, and CO for the subsequent analysis of the effects of the CAAA on health, agriculture, and the economy within the continental U.S. Although the CAAA applies to the entire nation, due to geographical considerations, the modeling domain includes the contiguous 48 states. The modeling was performed for a base year (1990) and for four future-year scenarios. The future-year scenarios include Post-CAAA and Pre-CAAA scenarios (the former incorporating emission changes associated with measures and programs pursuant to the CAAA) for the years 2000 and 2010. These years were selected to accommodate implementation schedules and time for effectiveness periods associated with many of the CAAA measures and programs.

Air Quality Models and Databases

To the extent possible, the section 812 prospective modeling analysis utilized existing modeling databases (from State Implementation Plan or other regional-scale modeling efforts). To accommodate the geographical extent and resolution required for this study, these included the input databases corresponding to both urban- and regional-scale applications of several different modeling systems. The lack of an existing comprehensive, fully tested, integrated modeling system (and associated databases) for use in this study precluded the integrated analysis of the various pollutants. This, however, may be an area for improving future prospective analyses.

The UAM and UAM-V modeling systems were applied to the analysis of the effects of the CAAA on ozone air quality. Specifically, the UAM-V modeling system was applied for the regional-scale analysis of ozone concentrations within both the eastern and western portions of the U.S. (separately). The analysis of the eastern U.S. relied upon the use of modeling databases developed as part of the Ozone Transport Assessment Group (OTAG) regional-scale modeling analysis. This modeling system was also applied for the western U.S., but at a relatively coarse resolution. To enhance the analysis for selected urban areas in the western U.S., the regional-scale modeling results were supplemented with higher-resolution modeling results for Los Angeles, Phoenix, and the San Francisco Bay Area. The results for both Los Angeles and Phoenix were obtained using the UAM modeling system, while those for the San Francisco Bay Area were obtained using the UAM-V modeling system.

The RADM/RPM and REMSAD modeling systems were used to estimate PM concentrations for the eastern and western U.S., respectively. Again, many of the inputs for application of these models were developed as part of other studies and adapted for use in the section 812 prospective modeling analysis.

As noted earlier, an emissions-based, linear "roll-back" technique was used to estimate future-year concentrations for SO_2, NO, NO_2, and CO. This approach was used for all areas of the continental U.S.

All of the modeling applications relied on the use of detailed estimates of emissions for the base year and each of the future-year scenarios. These are described by (Pechan, 1998). Modeling emission

inventories were prepared using the Emissions Preprocessing System (EPS2.5) (SAI, 1992).

Methodology for the Combined Use of Observations and Air Quality Modeling Results

The 812 prospective modeling analysis included several steps. First, concentration estimates for each pollutant of interest, corresponding to a base year of 1990, were prepared based on 1990 emissions and application of the appropriate modeling tool(s). For each scenario, the remaining steps consisted of (1) preparation of future-year, model-ready emission inventory estimates, (2) application of the appropriate modeling technique to estimate the change in air quality from the base year of 1990, (3) adjustment of the 1990 observed data to reflect the change as predicted by the modeling system, and (4) calculation of statistical quantities or "profiles" describing the predicted pollutant concentration distribution for each monitoring site.

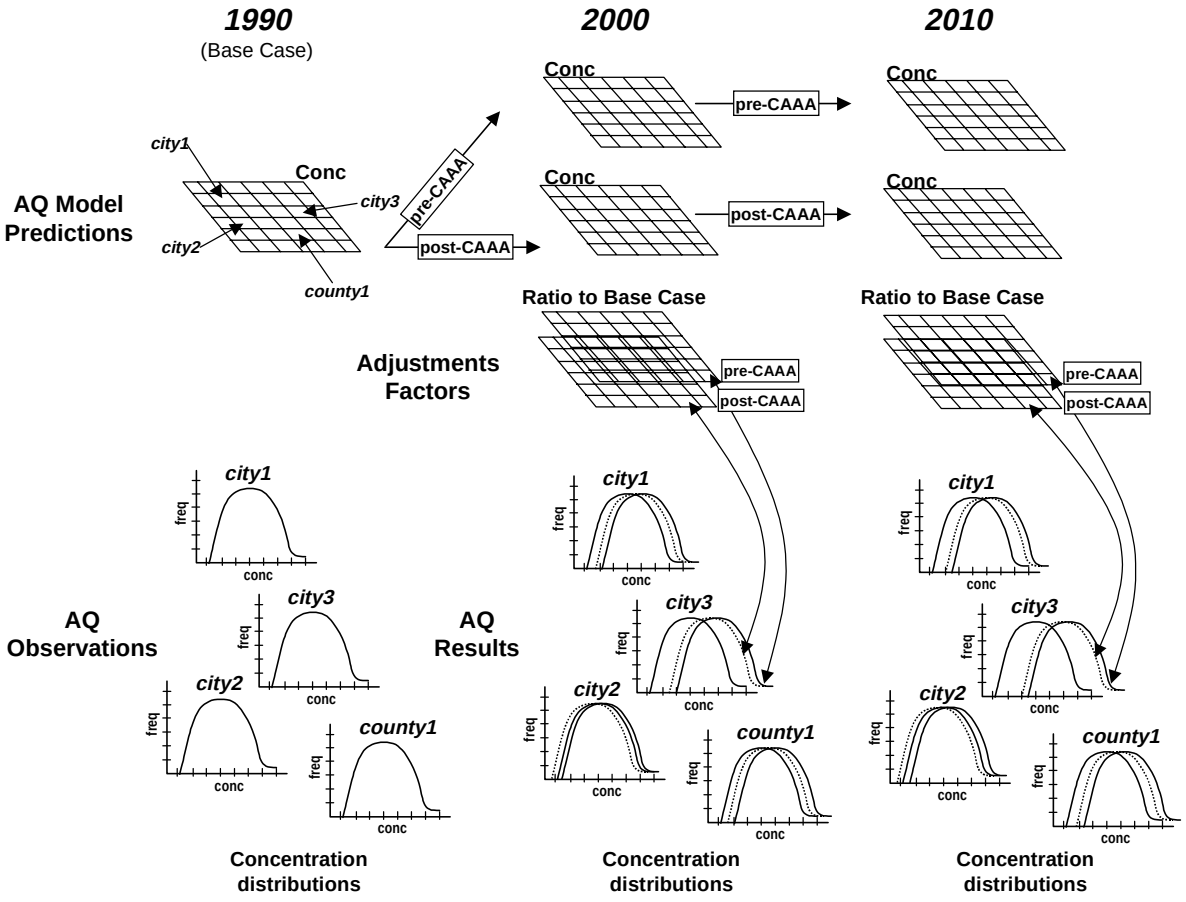
Conceptually, the methodology for estimating future-year ozone air quality using both observations and modeling results is rather simple. The modeling results are used to calculate adjustment factors for each monitoring site that is located within the modeling domain. This is done on a grid-cell by grid-cell basis (i.e., the adjustment factor for a monitoring site is based on the simulation results for the grid cell in which it is located). The adjustment factor represents the ratio of the future-year-scenario concentrations to the base-year concentrations and is calculated using appropriately matched values for several different concentration levels (i.e., the changes in concentration are dependent upon concentration level). The observed concentrations for each monitoring site are then modified using the site-specific (or grid-cell-specific) adjustment factors. The resulting values represent the estimated future-year concentrations.

This approach to estimating future air quality differs from that for a typical air quality model application (e.g., for ozone attainment demonstration purposes) in that the modeling results are used in a relative sense, rather than an absolute sense. This may enhance the reliability of the future-year concentration estimates, especially in the event that the uncertainty inherent in the absolute concentration values is greater than that associated with the response of the modeling system to changes in emissions.

Although the ratios are calculated using modeling results for a limited number of simulation days, it is assumed, using this methodology, that the ratios can be used to represent longer time periods. Consequently, all observations contained within the dataset (a few exceptions are discussed later in this document) are adjusted using the model-derived ratios. Thus, by applying the model-derived ratios to observed values representing longer periods, this approach also permits the estimation of seasonal and annual concentration distributions – a requirement for this study. Following the calculation of various n-hour rolling averages for each monitoring site, statistical quantities, or "profiles", describing the ozone distribution for each monitor are then calculated.

The future-year air quality profile estimation methodology, as applied to the analysis of results for the section 812 prospective analysis, is described in detail in the remaining sections of this document. A flowchart illustrating the methodology is provided in Figure C-1. The procedure makes use of the statistical functions and data handling capabilities of the Statistical Analysis Software (SAS) package.

Figure C-1
Schematic diagram of the future-year concentration estimation methodology.



[NOTE: Figure illustrates how model results and observations are used to produce air quality profiles (concentration distributions) for the benefits analysis. The figure shows model runs at the top; four sets of "ratios" of model results in space in the middle; and frequency distributions of pollutant monitor concentrations and the space-dependent scaling of these by the ratios of the model predictions on the bottom.]

Estimating the Effects of the CAAA on Ozone Air Quality

Future-year ozone concentrations corresponding to the Post-CAAA and Pre-CAAA scenarios were estimated through application of the UAM and UAM-V modeling systems. This section of the report contains an overview of the modeling systems and, for each geographical domain, a description of the application procedures and results. The calculation of ozone air quality profiles using the combined modeling results from the regional- and urban-scale modeling applications is also described.

For ease of reading, all figures follow the text in this section.

Overview of The UAM and UAM-V Photochemical Modeling Systems

UAM

The UAM is a three-dimensional photochemical grid model that calculates concentrations of pollutants by simulating the physical and chemical processes that occur in the atmosphere. It is formulated based on the atmospheric diffusion or species continuity equation. This equation represents a mass balance that includes all of the relevant emissions, transport, diffusion, chemical reaction, and removal processes in mathematical terms. The UAM incorporates the Carbon Bond IV chemical mechanism, which groups pollutant species to limit the number of chemical reactions, while permitting reasonable accuracy in simulating ozone and its precursors.

The major factors that affect photochemical air quality include:

- spatial distribution of emissions of volatile organic compounds (VOC) and NO_x, both natural and anthropogenic,
- composition of the emitted VOC and NO_x,
- spatial and temporal variations in the wind fields,
- dynamics of the boundary layer, including stability and the level of mixing,
- chemical reactions involving VOC, NO_x, and other important species,
- diurnal variations of solar insolation and temperature,
- loss of ozone and ozone precursors by dry and wet deposition, and
- ambient background concentration of VOC, NOx, and other species in, immediately upwind, and above the region of study.

The UAM simulates all of these processes. The species continuity equation is solved using the following fractional steps: emissions are injected; horizontal advection/diffusion is calculated; vertical advection/diffusion and deposition are calculated; and chemical transformations are performed for reactive pollutants. The UAM performs these four calculations during each time step. The maximum time step is a function of the grid size and the maximum wind velocity and diffusion coefficient. The typical time step is 10-15 minutes for coarse (10-20 km) grids and a few minutes for fine (1-2 km) grids.

Because it accounts for spatial and temporal variations as well as differences in the reactivity of emissions, the UAM is ideal for evaluating the air-quality effects of emission control scenarios. This is achieved by first replicating a historical ozone episode to establish a base-case simulation. Model inputs are prepared from observed meteorological, emissions, and air quality data for the episode days using prognostic meteorological modeling and/or diagnostic and interpolative modeling techniques. The model is then applied with these inputs, and the results are evaluated to determine model performance. Once the model results have been evaluated and determined to perform within prescribed levels, the same base-case meteorological inputs are combined with *modified* or *projected* emission inventories to simulate possible alternative/future emission scenarios.

The current UAM modeling system was released by the EPA in 1990 and is fully documented in the UAM user's guide (SAI, 1990). Features of the modeling system include a mixing-height-based vertical coordinate system and flux- and process-analysis capabilities to facilitate the comprehensive assessment of model performance and the interpretation of simulation results.

UAM-V

The UAM-V modeling system represents an extension of the UAM. Like UAM, the UAM-V incorporates the Carbon Bond IV chemical mechanism. Other features of the UAM-V modeling system include:

- *Variable vertical grid structure:* The structure of vertical layers can be arbitrarily defined. This allows for higher resolution near the surface and facilitates matching with output from prognostic meteorological models.

- *Three-dimensional meteorological inputs:* The meteorological inputs for UAM-V vary spatially and temporally. These are usually calculated using a prognostic meteorological model.

- *Variable grid resolution for chemical kinetic calculations:* A chemical aggregation scheme can be employed, allowing chemistry calculations to be performed on a variable grid while advection/diffusion and emissions injections are performed on a fixed grid.

- *Two-way nested grid:* Finer grids can be imbedded in coarser grids for more detailed representation of advection/diffusion, chemistry, and emissions. Several levels of nesting can be accommodated.

- *Updated chemical mechanism:* The original Carbon Bond IV chemical mechanism has been updated to include the XO_2/RO_2 reaction, along with new temperature effects for PAN reactions. Aqueous-phase chemistry is also an option.

- *Dry deposition algorithm:* The dry deposition algorithm is similar to that used by the Regional Acid Deposition Model (RADM).

- *True mass balance:* Concentrations are advected and diffused in the model using units of mass per unit volume rather than parts per million. This maintains true mass balance in the advection and diffusion calculations.

- *Plume-in-grid treatment:* Emissions from point sources can be treated by a subgrid-scale Lagrangian photochemical plume model. Pollutant mass is released from the subgrid-scale model to the grid model when the plume size is commensurate with a grid cell size.

- *Plume rise algorithm:* The plume rise algorithm is based on the plume rise treatment for a Gaussian dispersion model.

Regional-Scale Modeling of the Eastern U.S.

For this study, the UAM-V modeling system was applied separately for the eastern and western portions of the U.S. For the eastern U.S., the application was based, in part, on the regional-scale modeling analysis conducted by the Ozone Transport Assessment Group (OTAG). With the exception of the emission inventories, all inputs were those used for the OTAG modeling analysis. The application procedures and modeling results are summarized in this section.

UAM-V Application Procedures for the Eastern U.S.

Modeling Domain

The modeling domain for application to the eastern U.S. is identical to that used for the OTAG modeling analysis. The domain encompasses the 37 eastern most states and the District of Columbia and consists of two grids. The horizontal resolution for the outer grid is approximately 36 km; this grid consists of five vertical layers. The horizontal resolution for the smaller inner grid is approximately 12 km; this grid consists of seven vertical layers. The top of the modeling domain is 4000 meters above ground level.

Simulation Periods

Two of the OTAG multi-day simulation periods were selected for use in this study. These are 20-30 July 1993 and 7-18 July 1995. Both simulation periods are characterized by high ozone concentrations in the eastern U.S.; numerous exceedances of the 1-hour National Ambient Air Quality Standard (NAAQS) for ozone were recorded. During the 1993 simulation

period, the exceedances occurred mostly within the southeastern U.S. During the 1995 period, high ozone concentrations were observed in several regions including the Lake Michigan area, the Northeast Corridor, and the Southeast. These periods were chosen to be representative of regional-scale ozone transport events for the southeastern and eastern U.S. respectively. In both cases, the extent of the high ozone concentrations is attributable to persistent, regional-scale ozone conducive meteorological conditions. The simulation periods include two and three initialization (or start-up) days, respectively. These are included to reduce the effects of uncertainties in the initial conditions on the simulation results.

Input Preparation

The UAM-V modeling system requires a variety of input files that contain information pertaining to the modeling domain and simulation period. These include gridded, day-specific emissions estimates and meteorological fields; initial and boundary conditions; and land-use information.

Separate emission inventories were prepared for the base-year and each of the future-year scenarios. All other inputs were specified for the base-year model application (1990) and remained unchanged for each future-year modeling scenario.

Modeling Emission Inventories

The UAM-V requires detailed emission inventories containing temporally allocated emissions for each grid cell in the modeling domain and for all primary pollutant species represented by the chemical mechanism. An extended version of EPA's UAM Emissions Preprocessor System, Version 2.0, or EPS 2.0 (SAI, 1992) called EPS 2.5e was used to process the inventories. In addition to the capabilities of EPS 2.0, this system has been enhanced to facilitate regional-scale model applications of particulate matter and toxic species, as well as ozone precursors.

Each inventory includes weekday/weekend area source emissions, typical summer day utility emissions, weekday/weekend non-utility point source emissions, and day-specific biogenic emissions. The on-road motor-vehicle emissions were based on typical summer weekday/weekend estimates.

Anthropogenic input emissions inventory data were provided by Pechan (1998). These included area and point source emissions data from the National Particulates Inventory (by county and for specific point sources), county-level vehicle miles traveled (VMT) estimates, and mobile-source emission factors for VOC, NO_x, and CO. Area source emissions include emissions from a variety of sources such as commercial and residential fuel combustion, non-point-source industrial emissions, solvent utilization, construction equipment, off-highway vehicles, gasoline distribution, furniture refinishing, and lawn mowers. Day-specific, model-ready biogenic emission inventories were obtained from the OTAG database. Preparation of the emission inventory data is described in detail by Pechan (1998). A brief description of the emissions processing is provided in this section.

Preliminary processing of the data prior to the application of the EPS 2.5e system was necessary. This consisted of generating the on-road mobile emissions and reformatting all data into Atmospheric Information Retrieval System (AIRS) Mobile-Source Subsystem (AMS) and Facility Subsystem (AFS) work-file formats. On-road mobile emissions were generated using the inputs provided by EPA and the MOBILE5a model. The outputs from MOBILE5a include future-year emissions of the ozone precursor pollutants VOC, NO_x, and CO. MOBILE5a accesses a matrix of emissions factors that are based on temperature, speed, and other site-specific parameters. Estimates of VMT were multiplied by emission factors to generate on-road motor vehicle emission estimates. The VMT estimates were provided at county level and were broken down into 12 different urban and rural roadway classifications.

All anthropogenic emission inputs to UAM-V were preprocessed through the EPS 2.5e emissions processing system. Photochemical grid models such as the UAM-V require detailed emission inventories, containing hourly emissions for each grid cell in the modeling domain for each species being simulated. The core EPS system is a series of FORTRAN modules that incorporate spatial, temporal, and chemical resolution into an emissions inventory used for photochemical modeling. Point, area, and mobile source emission data were processed separately to facilitate both data tracking for quality control and the use of the data in evaluating the effects of alternative control strategies on simulated air pollutant concentrations. The mobile source component was further broken down into rural and urban motor vehicle emissions based on the roadway classifications. The model-ready components (including biogenic) were then merged to generate the final model inputs.

The UAM-V requires hourly estimates of emissions for each grid cell to accurately simulate hourly concentrations of ozone. Accordingly, annual average or peak ozone season daily emission rates must be adjusted to reflect the conditions of the ozone episode being modeled, including seasonal adjustments for activity levels (if base year emissions are reported as annual averages), adjustments for the day of the week, and hourly temperature and activity adjustments for each hour of the episode day. EPA has developed a default set of temporal allocation factors (TAF) for each source category and these have been incorporated into EPS 2.5e. TAF were applied to all model inputs. For the eastern U.S. domain, the available typical peak ozone season day NO_x and VOC emissions were adjusted for day of week and hourly allocation.

The Carbon-Bond IV chemical mechanism employed by the UAM-V modeling system, groups or "lumps" pollutants to limit the number of reactions and species to a reasonable level while permitting reasonable accuracy in predicting air quality. Ozone precursor hydrocarbon emissions were aggregated into the carbon-bond species required by the UAM-V using speciation profiles developed by the EPA (1991) and the default assignments provided with EPS. The chemical speciation scheme for VOCs includes eight categories: olefins, paraffins, toluene, xylene, formaldehyde, higher aldehydes, ethenes, and isoprene. For this study, the default NO_X speciation of 90 percent NO and 10 percent NO_2 by weight, included in EPS 2.5e, was assumed for all point and area sources.

For the UAM-V model to accurately simulate observed air quality concentrations for the selected grid, it must be supplied with emissions data that have the same degree of spatial resolution (i.e., by grid cell). The effort required to implement this resolution varies depending on the type of source. For point sources, geographical coordinates for each source, typically reported to within a fraction of a kilometer, are used for direct assignment of emissions to the appropriate grid cells. By contrast, spatial resolution of emissions reported as county totals, as is usually the case for area sources and motor vehicles, requires substantially more effort. The most commonly employed approach for apportioning county-level emissions to grid cells is to use a surrogate indicator for spatial distribution of emission levels or activity (e.g., population, type of land use, or location of major links such as interstate roadways or airport runways). A spatial allocation surrogate is a quantity whose areal distribution is either known or has been estimated and is assumed to be similar to the areal distribution of emissions from some source category whose spatial distribution is not well known. County-level emissions are spatially allocated to the grid cells of the modeling domain. Surrogate data input used to create the spatial allocation factors included U.S. Geological Survey (USGS) land-use data, 1990 census data, and digitized county boundaries.

Emissions totals by component for VOC, NO_x, and CO for the base- and future-year scenarios are provided in Table C-1. This table shows increases in VOC and NO_x under the Pre-CAAA scenarios and substantial decreases under the Post-CAAA scenarios. The decreases in VOC are primarily attributable to reductions in area- source and motor-vehicle emissions. The decreases in NO_x are due to decreases in motor-vehicle and utility and non-utility point-source emissions.

Air Quality, Meteorological, and Land-Use Inputs

The air quality, meteorological, and land-use inputs for application of the UAM-V modeling system for this study were identical to those used for the OTAG modeling exercise. The initial and boundary concentrations for the OTAG simulations were represented by "clean" air values for all species. The individual species concentrations vary slightly with elevation (or height above the ground) and with time of day, and are approximately 0.1 parts per billion (ppb) of NO_x, 5 parts per billion carbon (ppbC) of reactive hydrocarbons (RHC), and 100 ppb of CO. The boundary concentrations for ozone range from about 31 to 34 ppb. Further detail on the OTAG initial and boundary concentrations has been presented in OTAG publications (e.g., Deuel et. al., 1996).

Other input data required by the UAM-V model for simulating the ozone episodes (including the meteorological and land-use inputs) were obtained directly from the OTAG datasets without modification. Model options were the same in the current application as in the OTAG application, except that the plume-in-grid (P-i-G) treatment (a detailed treatment of the chemistry and geometry of plumes from elevated point sources) was not employed. This exception was made in order to reduce the demands on computer resources.

Table C-1
Emission Totals by Component for each Scenario for the OTAG Domain (tpd)

			VOC		
	Base 1990	**2000 Pre-CAAA**	**2000 Post-CAAA**	**2010 Pre-CAAA**	**2010 Post-CAAA**
Area	33,417	38,517	27,982	43,113	8,638
Onroad Mobile	17,518	15,102	10,074	17,400	8,552
Point	8,247	9,027	7,317	10,194	8,204
Utility	87	81	82	111	113
Total	**59,270**	**62,727**	**45,454**	**70,818**	**45,507**
			NOx		
	Base 1990	**2000 Pre-CAAA**	**2000 Post-CAAA**	**2010 Pre-CAAA**	**2010 Post-CAAA**
Area	12,109	13,858	13,351	15,770	13,741
Onroad Mobile	17,915	17,463	14,923	20,222	12,616
Point	6,647	7,345	4,444	8,365	4,681
Utility	17,637	20,668	8,254	22,670	5,182
Total	**54,307**	**59,335**	**40,972**	**67,026**	**36,220**
			CO		
	Base 1990	**2000 Pre-CAAA**	**2000 Post-CAAA**	**2010 Pre-CAAA**	**2010 Post-CAAA**
Area	46,606	53,087	51,544	58,952	57,100
Onroad Mobile	147,842	112,656	84,569	124,385	78,396
Point	13,766	15,463	15,463	17,192	17,192
Utility	710	784	811	1,225	1,327
Total	**208,924**	**181,990**	**152,388**	**201,753**	**154,015**

UAM-V Simulation Results for the Eastern U.S.

Model Performance

The assessment of model performance is an important component of a modeling analysis and is used to ensure that the modeling system, including the inputs, is able to replicate the observed concentration levels associated with the historical modeling episode period. The evaluation of model performance is typically achieved through the comparison of simulated concentrations with observed data. In this case, the observed data correspond to the actual episode period and the emissions reflect emission levels for that same period/year. For the OTAG modeling component, model performance considered the base-case applications for 1993 and 1995.

Model performance for the OTAG episodes is documented in the OTAG modeling report (OTAG, 1997). In general, the observed ozone concentration levels were represented in the simulations, with some over- and under-estimation of the maximum values. Scatter plots comparing the simulated and observed concentrations for key modeling days for each episode (28 July 1993 and 15 July 1995) show generally good agreement between the simulated and observed values, with some tendency for over- and underestimation on all days, distributed among the concentration levels (scatter along the axis). These are typical of the comparisons for the other simulation days.

Since the simulation results corresponding to all concentration levels will be used to adjust the observed data for Section 812 modeling analysis a comparison of the mean values was also performed. Plots comparing the mean values for each simulation day of the 1993 and 1995 simulation periods in both cases show that the mean simulated values are slightly higher than the mean observed values, but the day-to-day tendencies are similar.

For the 1993 simulation period, the mean unsigned relative error (or normalized bias) ranges from approximately -15 percent to 1 percent. The corresponding values for the 1995 simulation period are -12 to 9 percent. These are all within the EPA recommended range (for urban-scale modeling) of ±15 percent. For both simulation periods, the mean relative error (or gross error) is less than 25 percent for each simulation day. The EPA recommended range is less than 35 percent.

The good agreement between the simulated and observed ozone concentrations, suggests that the OTAG modeling system (including the meteorological, air quality, and geographical inputs) provides an appropriate basis for the Section 812 prospective modeling.

UAM-V Modeling Results

The UAM-V simulation results for the Pre- and Post-CAAA scenarios were used in this study to calculate factors for adjustment of observed data and estimation of future-year concentration levels. These were calculated by comparing the simulated concentrations corresponding to each future-year/scenario simulation with those for the base-year simulation (1990). Examples of this comparison are illustrated using isopleth plots for maximum ozone concentration in Figures C-2 and C-3.[1] These isopleth plots correspond to 1995 simulation period and depict differences in maximum ozone concentration for 15 July between the 1990 baseline and the 2010 Pre- and 2010 Post-CAAA scenarios, respectively. The differences are calculated as scenario minus base, so that negative values indicate lower concentrations for the future-year scenario. These plots indicate that for 2010 the Pre-CAAA simulation results are characterized by increases in ozone, while the Post-CAAA results show decreases in ozone. Similar results were found for both future years and for both episodes modeled (SAI, 1999). The increases occur over the mid- and southern sections of the domain while the decreases are more widespread. Both the

[1]For many of the figures in this appendix the Pre-CAAA scenario and Post-CAAA Scenario are referred to as Pre-CAAA90 and post CAAA90, respectively.

increases and decreases are larger and more widespread for 2010.

It is also useful to directly compare the Pre- and Post-CAAA simulation results for each future year. This gives a direct indication of the effects of the CAAA on the simulated ozone concentrations. For example, Figure C-4 illustrates the differences in maximum simulated ozone concentration between the Pre- and Post-CAAA simulations for 2010 for the 15 July 1995 simulated ozone episode. The differences are calculated as Post-CAAA minus Pre-CAAA, so that negative values indicate lower concentrations for the Post-CAAA scenario. In general the results of these comparisons indicate that except for isolated increases (single grid cells), the simulated daily maximum ozone concentrations for the Post-CAAA scenario are lower than the corresponding Pre-CAAA values for both future years. The spatial extent of the decreases is greater for 2010.

Regional-Scale Modeling of the Western U.S.

Application of the UAM-V modeling system to the western U.S. utilized inputs from the regional-scale application of REMSAD (as described in the next section of this report). The objective of this application was to provide regional-scale ozone concentration estimates for those areas that are neither included in the OTAG domain nor in the urban-scale analyses. The application procedures and modeling results are summarized in this section.

UAM-V Application Procedures for the Western U.S.

Modeling Domain

The modeling domain used to obtain results for the western U.S. is identical to that used for application of the REMSAD modeling system (as described in the following section of this report) for the PM-related analysis of the CAAA. The modeling domain encompasses the contiguous 48 states, extending from 126 degrees west longitude to 66 degrees west longitude, and from 24 degrees north latitude to 52 degrees north latitude. A grid cell size of 2/3 longitude by 1/2 latitude (approximately 56 by 56 km) results in a 90 by 55 grid (4,950 cells) for each vertical layer. Eight vertical layers were used. Note that although the domain includes the entire contiguous 48 states, results using this domain configuration were only used to estimate ozone concentrations for the western states.

Simulation Period

For the western U.S., the simulation period included 1-10 July 1990. As noted earlier, this simulation period was selected to accommodate use of the REMSAD inputs and, therefore, represents the summertime simulation period for PM modeling of the western U.S. This period is characterized by high ozone concentrations (in excess of the 1-hour ozone NAAQS) in the Los Angeles area on all days, and in the San Joaquin Valley on 9 and 10 July. Relatively high concentrations were also observed in the San Francisco Bay Area, the Sacramento Valley, the San Diego area, and Denver. Throughout the remainder of the domain, concentrations typically did not exceed 100 ppb. The simulation period includes three initialization (or start-up) day that were included to limit the influence of the initial conditions on the simulation results.

Input Preparation

Preparation of the model-ready emission inventories for this application utilized the same data and followed the same procedures outlined in the previous section of this report. Emissions totals for the base- and future-year scenarios are provided in Table C-2 for VOC, NO_x, VOC, and CO.

The meteorological, air quality, and land-use related inputs were identical to those used for the application of the REMSAD modeling system to the western U.S. The reader is referred to Section 4 of this report for a description of these inputs and input preparation procedures.

Table C-2
Emission Totals by Component for each Scenario for the Entire U.S. (tpd).

			VOC		
	Base 1990	**2000 Pre-CAAA**	**2000 Post-CAAA**	**2010 Pre-CAAA**	**2010 Post-CAAA**
Area	33,972	39,154	27,620	43,708	28,575
Onroad Mobile	18,659	16,454	10,683	18,776	8,804
Point	9,503	10,298	8,457	11,606	9,454
Utility	96	85	85	134	137
Total	**62,229**	**65,991**	**46,845**	**74,224**	**46,970**
			NOx		
	Base 1990	**2000 Pre-CAAA**	**2000 Post-CAAA**	**2010 Pre-CAAA**	**2010 Post-CAAA**
Area	13,766	15,659	15,252	17,697	15,794
Onroad Mobile	20,399	20,660	17,421	24,142	14,696
Point	7,964	8,694	5,645	9,803	5,985
Utility	20,188	22,787	11,170	24,808	10,319
Total	**62,316**	**67,800**	**49,487**	**76,450**	**46,793**
			CO		
	Base 1990	**2000 Pre-CAAA**	**2000 Post-CAAA**	**2010 Pre-CAAA**	**2010 Post-CAAA**
Area	70,069	80,679	79,155	90,198	88,240
Onroad Mobile	171,181	142,346	103,332	153,706	92,058
Point	16,478	18,257	18,257	20,210	20,210
Utility	861	796	804	1,243	1,269
Total	**258,589**	**242,078**	**201,547**	**265,357**	**201,777**

UAM-V Simulation Results for the Western U.S.

Model Performance

Model performance for ozone was assessed for the entire western region and for five subregions. Model performance was evaluated through graphical comparison of the simulated and observed regional and subregional maximum ozone concentration patterns and values. Quantitative measures of model performance were calculated on a subregional basis, although typical model performance criteria are not applicable for the grid resolution and domain scale used for this analysis. Overall, the results indicate that ozone concentrations in the western U.S. are somewhat underestimated, relative to the observed values. On a subregional basis, the results vary from day to day and can be characterized as follows:

- Southern California Coast: Gross concentration gradients are directionally represented in the simulation results, with lower values along the coast and higher ozone inland. However, the resolution is not sufficient to

resolve even the higher values within the Los Angeles Basin. The maximum simulated value on any day is 83 ppb, while the maximum observed value exceeds 100 ppb (at a number of the sites within the region) on any given day of the simulation period. Results corresponding to Los Angeles were not used in subsequent portions of the analysis.

- Northern California/Southern Oregon/Central and Western Nevada: Simulated ozone concentrations tend to be lower than observed in the Sacramento Valley and San Joaquin Valley as well as (toward the end of the simulation period) the eastern portion of the San Francisco Bay Area. Daily maximum simulated ozone concentrations in the San Joaquin Valley range from approximately 60 to 86 ppb. Observed values greater than or equal to 100 ppb were recorded during 7-10 July. Representation of the observed concentration pattern improves throughout the simulation period. Concentrations at monitors in Oregon and Nevada are generally well represented. Results corresponding to northern California were not used in the subsequent analysis.

- Pacific Northwest/Eastern Washington: Low observed ozone concentrations are slightly to moderately overestimated through 7 July and underestimated (in some cases just slightly) for 8-10 July. For days with ozone concentrations greater than 40 ppb, the normalized bias ranges from approximately -12 to 20 percent. The normalized gross error is less than about 38 percent.

- Four Corners States: Maximum ozone concentration in Phoenix, Las Vegas, and Salt Lake City are reasonably well represented in the simulation results. Concentrations for the Denver are consistently underestimated. Those for Albuquerque and El Paso are well represented for certain of the days and underestimated for others. There are also a few isolated sites for which maximum ozone is reasonably well simulated (the observed concentrations are low). The normalized bias ranges from approximately -5 to 14 percent. The normalized gross error is less than 40 percent. Results for Phoenix were not used in the subsequent analysis.

- Montana/Idaho/Wyoming/ Western Portion of Dakotas: Day-to-day differences in concentrations are not well represented, however, the simulated values are generally consistent with the limited observations. The normalized bias ranges from zero to approximately 30 percent. The normalized error is greater than 35 percent for four of the simulation days.

- Note on the Eastern U.S.: Maximum simulated ozone concentrations range from approximately 160 to 250 ppb during the simulation period. Simulated peaks occur over Baton Rouge, Houston, St. Louis, and Atlanta with some high values along the NE corridor. These values have not yet been compared with observations, but simulated ozone concentrations are much higher in the east than in the west.

In general, the coarse resolution limits the ability of the modeling system to resolve peak concentrations and, in some cases, concentration gradients (such as those that occur along the coast of California). Based on these results, it was decided that the western ozone modeling results could be used to characterize the regional-scale concentration changes but would be supplemented with higher resolution modeling for Los Angeles, the San Francisco Bay Area (and portions of northern California), and Phoenix.

Simulated and observed concentrations for two of the modeling days (4 and 8 July 1990) were compared by SAI (1999). The differences between the simulated and observed values are typically larger than those for the OTAG simulations (possibly due to the coarser grid resolution) and represent both under- and overestimation of the maximum observed

concentrations. Underestimation of the higher concentrations is prevalent for nearly all of the simulation days.

In addition, a comparison of mean simulated and observed values by SAI showed that, while the highest values are underestimated, the mean simulated values are slightly greater than the observed means (SAI, 1999).

The model performance evaluation for the western ozone modeling application suggests that the modeling results can be used for the regional-scale analysis. Although the peak concentrations tend to be underestimated, there is not a uniform bias in the representation of the daily maxima. In addition, the mean values are fairly well characterized.

UAM-V Modeling Results

The UAM-V simulation results corresponding to the Pre- and Post-CAAA scenarios for 2010 are compared to the base-year values in Figures C-5 and C-6, respectively. The isopleth plots depict the differences in maximum ozone concentration for 8 July between the base (1990) simulation and the 2010 Pre- and Post-CAAA simulations, respectively. The differences are calculated as scenario minus base, so that negative values indicate lower concentrations for the future-year scenario. Similar results were found for both future years modeled (SAI, 1999) and indicate increases in daily maximum ozone for large portions of the western U.S. with smaller areas of decrease (e.g., over California) for the Pre-CAAA scenario. For the Post-CAAA scenarios, the plots indicate widespread decreases with small areas of increase.

A comparison of the Pre- and Post-CAAA simulation results for 2010 is provided in Figure C-7. The differences are calculated as Post-CAAA minus Pre-CAAA, so that negative values indicate lower concentrations for the Post-CAAA scenario. This comparison indicates lower ozone concentrations for the Post-CAAA scenario compared to the Pre-CAAA scenario over most of the western U.S., with some increases in the San Francisco Bay Area, Los Angeles, and Seattle. The simulation results suggest that NO_x reductions within these areas are disbeneficial with respect to ozone air quality. This is likely attributable to the reduced ozone titration that occurs in the simulation when NO_x emissions are reduced. This phenomenon is most frequently apparent in area where NO_x emissions are large relative to VOC emissions (VOC-limited areas).

Urban-Scale Modeling of the San Francisco Bay Area

High-resolution, urban-scale modeling of the San Francisco Bay Area (northern California) was intended to provide an improved basis (compared to the regional-scale application of UAM-V for the western U.S.) for the estimation of future-year ozone profiles for the Bay Area and portions of northern California. With the exception of the emission inventories, all inputs for this application were obtained from the Bay Area Air Quality Management District (BAAQMD), and used by permission. The application procedures and modeling results are summarized in this section.

UAM-V Application Procedures for the San Francisco Bay Area

Modeling Domain

The modeling domain for this application of the UAM-V modeling system includes the San Francisco Bay Area, the Monterrey Bay Area, Sacramento, and a portion of the San Joaquin Valley. The location and geographical extent of the domain is illustrated in Figure C-8. The domain consists of 102 by 102 horizontal grid cells with a grid spacing of 4 km. It also includes 16 vertical layers.

Simulation Period

The simulation period for the application to northern California is 3-6 August 1990. This episode period occurred during the San Joaquin Valley Air Quality Study and was characterized by moderate to

high ozone concentrations in the San Francisco Bay Area on 5 and 6 August, and in the Sacramento area and the San Joaquin Valley on 4, 5, and 6 August. The observed peak in the Bay Area was 120 ppb, while that for the other two more inland areas reached 150 ppb. The simulation period includes one initialization (or start-up) day that was included to limit the influence of the initial conditions on the simulation results.

Input Preparation

Preparation of the model-ready emission inventories for this application utilized the same data and followed the same procedures outlined in the previous section of this report. Emissions totals for the base- and future-year scenarios are provided in Table C-3 for VOC, NO_x, and CO. This table indicates a downward trend in emissions (between 1990 and 2000) followed by an upward trend (between 2000 and 2010) for the Pre-CAAA scenario. The increases are attributable to area- source and motor-vehicle emissions (i.e., increases in population and vehicle miles traveled). Emissions for both future years are lower than the base-year for the Post-CAAA scenario. The decreases are primarily due to a reduction in motor-vehicle emissions.

The meteorological, air quality, and land-use related inputs were prepared by the BAAQMD for use in their SIP modeling analysis. Documentation of the input preparation procedures and resulting inputs is available on-line (BAAQMD, 1998). Initial and boundary conditions for the future-year applications were estimated based on the corresponding emission reductions for VOC and NO_x; for ozone the square root of the product of the VOC and NO_x reduction factors was used.

Table C-3
Emission Totals by Component for each Scenario for the San Francisco Bay Area (tpd)

		VOC			
	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	783	795	644	886	698
Onroad Mobile	900	572	223	680	97
Point	111	110	110	110	93
Utility	1	0	0	1	1
Total	**1,795**	**1,477**	**977**	**1,677**	**889**
		NOx			
	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	381	407	392	458	396
Onroad Mobile	850	827	545	1,014	337
Point	202	197	140	197	140
Utility	46	4	4	2	2
Total	**1,479**	**1,435**	**1,081**	**1,671**	**874**
		CO			
	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	1,846	2,113	2,098	2,411	2,394
Onroad Mobile	7,414	5,652	2,526	6,630	1,444
Point	123	119	119	119	119
Utility	46	9	10	26	26
Total	**9,429**	**7,893**	**4,753**	**9,186**	**3,983**

UAM-V Simulation Results for the San Francisco Bay Area

Model Performance

Model performance was evaluated by the BAAQMD as part of their SIP modeling analysis and the inputs (with the exception of the modeling emission inventories) were used directly for the 812 prospective modeling analysis. Sscatter plots comparing the maximum simulated and observed ozone concentrations for both simulation periods are available in (SAI, 1999). These comparisons indicate good agreement between the simulated and observed values with a tendency for underestimation of the high observed ozone concentrations. Mean values are underestimated by about 10 to 15 percent on all days, which is within the current EPA range for acceptable urban-scale model performance (SAI, 1999).

Since good model performance is achieved, results of the model performance evaluation for ozone suggest that the UAM-V modeling platform for northern California (including the meteorological, air quality, and geographical inputs) provides an appropriate basis for the Section 812 prospective modeling.

UAM-V Modeling Results

Comparison of the UAM-V simulation results for the Pre- and Post-CAAA scenarios with the base-year values indicates both increases and decreases in the simulated concentrations for the Bay Area , both of which are greater in magnitude and more widespread for the Post-CAAA scenario and for 2010. Isopleth plots for the Bay Area are available in (SAI, 1999).

A comparison of the Pre- and Post-CAAA simulation results for 2010 is provided in Figure C-9. The differences are calculated as Post-CAAA minus Pre-CAAA, so that negative values indicate lower concentrations for the Post-CAAA scenario. This comparison indicates that the CAAA results in higher daily maximum ozone in the Bay Area but lower ozone throughout the remainder of the domain. Similar results were obtained for 2000 (SAI, 1999). These results are qualitatively consistent with the regional-scale modeling results presented in the previous section of this report. However, the extent of the increases is more limited and the decreases are greater in the refined modeling. Note the increases occur in areas where the base-year ozone concentrations are low to very low.

Urban-Scale Modeling of the Los Angeles Area

High-resolution, urban-scale modeling of the Los Angeles area was intended to provide an improved basis (compared to the regional-scale application of UAM-V for the western U.S.) for the estimation of future-year ozone profiles for this area. With the exception of the emission inventories, all inputs for this application were obtained from the South Coast Air Quality Management District (SCAQMD), and used by permission. As noted earlier, modeling of this area was performed using the UAM modeling system. The model formulation is similar to that for the UAM-V modeling system, but lacks certain features that make UAM-V suitable for regional-scale applications. The application procedures and modeling results are summarized in this section.

UAM Application Procedures for the Los Angeles Area

Modeling Domain

Application of the UAM-IV for the Los Angeles area was based on modeling performed by SCAQMD, as reported in the 1994 Air Quality Management Plan (SCAQMD, 1994). The modeling domain for this application is a 65 by 40 array of 5 km resolution grid cells. The domain also contains 5 vertical layers. The domain encompasses the South Coast Air Basin (SoCAB) (from Los Angeles to beyond Riverside) and a portion of the Mojave Desert. The location and geographical extent of the domain is illustrated in Figure C-8.

Simulation Period

Two simulation periods were included in the modeling analysis for Los Angeles: 23-25 June 1987 and 26-28 August 1987. Both of these episodes occurred during the 1987 Southern California Air Quality Study (SCAQS). In both cases, the simulation period includes one initialization, or start-up, day (in order to reduce the influence of the somewhat uncertain initial concentrations on model results).

Input Preparation

Preparation of the model-ready emission inventories for this application utilized the same data and followed the same procedures outlined in a previous section of this report. Emissions totals for the base- and future-year scenarios are provided in Table C-4 for VOC, NO_x, and CO. The Post-CAAA scenarios are characterized by lower emissions than the base year and the Pre-CAAA scenarios. The differences are largely attributable to changes in the motor-vehicle emissions.

The meteorological, air quality, and land-use related inputs were prepared by the SCAQMD for use in their SIP modeling analysis. The reader is referred to SCAQMD (1994 and 1996) for detailed information on the input preparation procedures and resulting inputs. Initial and boundary conditions for

the future-year applications were estimated based on the corresponding emission reductions for VOC and NO_x; for ozone the square root of the product of the VOC and NO_x reduction factors was used.

Table C-4
Emission Totals by Component for each Scenario for Los Angeles (tpd)

VOC

	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	758	770	607	871	700
Onroad Mobile	1,179	999	410	1,168	213
Point					
Low Level	197	196	196	196	158
Elevated	1	3	3	2	2
Total	**2,135**	**1,968**	**1,216**	**2,237**	**1,073**

NOx

	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	450	467	453	529	463
Onroad Mobile	993	1,280	879	1,573	626
Point					
Low Level	216	186	139	186	139
Elevated	19	19	18	12	8
Total	**1,678**	**1,953**	**1,489**	**2,300**	**1,236**

CO

	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	1,142	1,302	1,286	1,515	1,495
Onroad Mobile	9,046	10,043	5,046	11,278	3,728
Point					
Low Level	208	197	197	197	197
Elevated	2	43	44	34	35
Total	**10,398**	**11,586**	**6,573**	**13,024**	**5,456**

UAM Simulation Results for the Los Angeles Area

Model Performance

Model performance was evaluated by SCAQMD as part of their SIP modeling analysis and the inputs (with the exception of the modeling emission inventories) were used directly for the 812 prospective modeling analysis. Comparisons of maximum simulated and observed concentrations for each of the simulation periods are available in (SAI, 1999). They indicate a tendency for underestimation of the high observed ozone concentrations. This underestimation

also shows up in the comparison of the mean values (SAI, 1999).

While the urban-scale results are much better than those obtained with the coarser-resolution grid, both the maximum and mean values are underestimated. For the primary episode days, the normalized bias exceeds the EPA recommended range, while the normalized gross error is within approximately 35 percent. While this does not preclude the use of these results for the 812 study, it should be noted that the simulated changes in ozone between the base- and future-year scenarios may be influenced by the lack of good model performance. Use of the simulation results in the relative sense (through the calculation of adjustment factors) should reduce the uncertainty, compared to use of the absolute values.

UAM Modeling Results

Comparison of the UAM-V simulation results for the Pre- and Post-CAAA scenarios with the base-year values shows large reductions in daily maximum ozone for all four future-year scenarios. Some increases in ozone are simulated for 2010 for the Pre-CAAA scenario; overall, the extent and magnitude of the reductions is greater for the Post-CAAA scenario for both years. Isopleth plots for the Los Angeles area are available in (SAI, 1999).

A comparison of the Pre- and Post-CAAA simulation results for 2010 is provided in Figure C-10. The differences are calculated as Post-CAAA minus Pre-CAAA, so that negative values indicate lower concentrations for the Post-CAAA scenario. This comparison indicates lower maximum ozone concentrations under the Post-CAAA scenario for both years. Small increases occur over the urban area; these are smaller in extent and magnitude than for the regional modeling application. Similar results were found for 2000 (SAI, 1999).

Urban-Scale Modeling of the Maricopa County (Phoenix) Area

High-resolution, urban-scale modeling of Maricopa County, Arizona (which includes the Phoenix urban area) was intended to provide an improved basis (compared to the regional-scale application of UAM-V for the western U.S.) for the estimation of future-year ozone profiles for this area. With the exception of the emission inventories, all inputs for this application were obtained from the Maricopa Association of Governments (MAG), and used by permission. As noted earlier, modeling of this area was performed using the UAM modeling system.

UAM Application Procedures for the Phoenix Area

Modeling Domain

The modeling domain for the application of the UAM modeling system to the Phoenix area encompasses the urbanized portion of Maricopa County, Arizona; this domain was based on that used for a previous application of UAM for the area (Douglas et al., 1994). The domain consists of a 44 by 33 array of 2 km grid cells and 5 vertical layers. The location and geographical extent of the domain is illustrated in Figure C-8.

Simulation Period

Two ozone episodes were also simulated for the Phoenix area: 9-10 August 1992 and 13-14 June 1993. Exceedances of the 1-hour NAAQS for ozone were recorded during both episodes. Each period also includes one initialization day.

Input Preparation

Preparation of the model-ready emission inventories for this application utilized the same data and followed the same procedures outlined in a previous section of this report. Emissions totals for the base- and future-year scenarios are provided in

Table C-5 for VOC, NO_x, and CO. The changes in emissions are characterized by both increases and decreases, reflecting an expected growth in population that is offset by fleet turnover and other emission reduction measures.

The meteorological, air quality, and land-use related inputs were prepared by Douglas et al. (1994). The reader is referred to this technical report for detailed information on the input preparation procedures and resulting inputs. Initial and boundary conditions for the future-year applications were estimated based on the corresponding emission reductions for VOC and NO_x; for ozone the square root of the product of the VOC and NO_x reduction factors was used.

UAM Simulation Results for the Phoenix Area

Model Performance

Model performance was evaluated by Maricopa Association of Governments (MAG) as part of their SIP modeling analysis and the inputs (with the exception of the modeling emission inventories) were used directly for the 812 prospective modeling analysis. Comparison of hourly simulated and observed ozone concentrations indicates good agreement between the simulated and observed values. Mean values are well represented as well. Plots of these comparisons are available in (SAI, 1999). For the primary modeling days, the normalized bias and error statistics indicate very good model performance. The values are less than 5 percent (bias) and 20 percent (error) respectively (SAI, 1999).

The model performance results indicate that the UAM modeling system (including the meteorological, air quality, and land-use input) are appropriate for use in the Section 812 prospective analysis.

UAM Modeling Results

Comparison of the UAM-V simulation results for the Pre- and Post-CAAA scenarios with the base-year values indicates both increases and decreases for the Pre-CAAA scenario simulations and large decreases for the Post-CAAA scenario simulations. Isopleth plots for the Phoenix area are available in (SAI, 1999).

A comparison of the Pre- and Post-CAAA simulation results for each future year indicates that the CAAA measures reduce daily maximum ozone concentrations within the Phoenix domain by approximately 10 to 20 ppb (more or less in some areas) for both future years. Isopleth plots for the Phoenix area are available in (SAI, 1999).

Table C-5
Emission Totals by Component for each Scenario for Phoenix (tpd)

VOC

	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	241	310	201	369	250
Onroad Mobile	184	215	141	231	85
Point					
Low Level	2	2	1	2	2
Elevated	0	0	0	0	0
Total	**426**	**527**	**344**	**602**	**337**

NOx

	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	213	270	259	326	290
Onroad Mobile	151	214	174	264	147
Point					
Low Level	1	1	1	2	2
Elevated	0	0	0	0	0
Total	**371**	**485**	**434**	**592**	**438**

CO

	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	684	820	795	941	907
Onroad Mobile	1,186	2,001	1,538	1,883	1,002
Point					
Low Level	0	0	0	0	0
Elevated	1	1	1	1	1
Total	**1,871**	**2,822**	**2,334**	**2,825**	**1,910**

Calculation of Ozone Air Quality Profiles

The overall objective of the photochemical modeling exercise was to provide estimates of future-year ozone air quality for 2000 and 2010 (for assessment of the effects of the CAAA). This was accomplished using an approach that combines observed data and air quality modeling results to estimate future-year concentrations. The methodology is designed to provide site-specific, seasonal and annual ozone concentration distributions. The statistical concentration distributions are estimated (based on the results of air quality modeling) for specific future-year scenarios and, in turn, provide the basis for examination and quantification of the effects of changes in air quality on health, agriculture, etc. (i.e., physical effects and economic valuation modeling). Through comparison with corresponding results for a baseline simulation (in this case without the CAAA measures and programs), the effects of the CAAA can be assessed. The future-year air quality profile estimation methodology, as applied to the analysis of the CAAA, is described in this section.

Overview of the Methodology

Conceptually, the methodology for estimating future-year ozone air quality using both observations and UAM-V simulation results is rather simple. The UAM-V simulation results are used to calculate adjustment factors for selected ozone monitoring sites within the modeling domain. This is done on a grid-cell by grid-cell basis (i.e., the adjustment factor for a monitoring site is based on the simulation ozone concentrations for the grid cell in which it is located). The adjustment factor represents the ratio of the future-year-scenario to the base-year concentrations and is calculated (using the appropriately matched values) for several different concentration levels (i.e., the changes in concentration are dependent upon relative concentration level). The observed ozone concentrations for each monitoring site are then modified using the site-specific (or grid-cell-specific) adjustment factors. The resulting values represent the estimated future-year ozone concentrations for the modeled scenario.

As noted earlier in this report, the overall approach to estimate future air quality differs from that for a typical air quality model application (e.g., for attainment demonstration purposes) in that the modeling results are used in a relative sense, rather than an absolute sense. This may enhance the reliability of the future-year concentration estimates, especially in the event that the uncertainty inherent in the absolute concentration values is greater than that associated with the response of the modeling system to changes in emissions. This approach also permits the estimation of seasonal and annual concentration distributions, a requirement for this study.

Although the ratios are calculated using modeling results for a limited number of simulation days, it is assumed, using this methodology, that the ratios can be used to represent longer time periods. Consequently, all observations contained within the dataset are adjusted using the model-derived ratios. Following adjustment of the observed data, statistical quantities, or "profiles", describing the ozone distribution for each monitoring site are then calculated.

Description of the Observation Dataset

One of the unique aspects of this approach to evaluating future ozone air quality is the use of observed ozone concentrations to supplement model results. As such, one of the earliest tasks was the creation of a dataset containing the observed hourly ozone concentrations for all monitoring sites located within the modeling domains for the months of May through September 1990.

Hourly ozone concentrations for 1990 were extracted from the Aerometric Information Retrieval System (AIRS) and input into a single AMP350-format datafile. From the information contained in this file, two SAS datasets were created: a concentration dataset and a monitor information dataset). The concentration dataset contains the

hourly concentrations for each monitor, with each record in the dataset representing a single monitor-day. The monitor information dataset contains monitor-specific information such as land-use and location.

In creating the concentration dataset, some data handling issues arose and were addressed in the following manner:

- In some instances, multiple ozone monitoring devices were operated at the same location. Even though these different devices have the same AIRS state-county-site identification code (ID), they are differentiated by a parameter occurrence code (POC). The AIRS state-county-site ID was concatenated with the POC to form a unique identifier for each monitor. A POC greater than 5 typically indicates that a device was being calibrated; information/data for these monitors was/were not included in either the monitor or the concentration dataset.

- In the AIRS database, ozone concentrations are reported using the default unit of the reporting agency. Thus, multiple units were present in the AMP350 file. For ease of analysis, all of the concentrations were converted to a single unit, ppm.

- Missing ozone concentrations in the AIRS AMP350 report are indicated by a blank in the decimal field. In the concentration dataset for this study, the SAS missing value code was used to indicate missing data.

- For each monitor a method detection limit (MDL) was provided. The MDL indicates a threshold below which reported ozone concentrations do not accurately reflect the sample distribution. For most monitors the MDL is 0.005 ppm. Because this value is low relative to typical ambient concentration levels, observed values below the MDL were not reset to the MDL and instead were left unchanged.

Only monitors with "complete" data were used in the analysis. For the ozone data, a monitor record was considered to be complete if data were available for 50 percent of the days in the peak ozone season (May-September). Each of these days in turn had to have at least 12 hourly observations. There were 842 ozone monitors with complete data.

Calculation of Percentile-Based Adjustment Factors

For each future-year modeling scenario, grid-cell-specific adjustment factors were calculated using the hourly simulated ozone concentrations contained in the UAM-V or UAM *xymap*[2] output files. Individual monitoring sites were mapped onto the gridded model output (to determine the grid cell in which each monitor was located) and the concentrations for the corresponding grid cells were used to calculate a set of ten adjustment factors for each future-year modeling scenario. The adjustment factors were specified to be the ratio of the percentile concentrations for the future- and base-year simulations, where the percentile concentrations were calculated using data for each hour of each simulation day:

$$Adjustment\ Factor_i = \frac{x_i th\ Percentile\ \ Concentration_{future\ year}}{x_i th\ Percentile\ \ Concentration_{base\ year}}$$

$$\{x_i\} = \{5, 15, 25, 35, 45, 55, 65, 75, 85, 95\}$$

For calculation of the percentile concentrations, the empirical distribution function with averaging was employed. Because the concentrations for the lower percentiles can be rather small, a threshold value of 1 ppb was set to keep the adjustment factors reasonable. In other words, all concentrations below 1 ppb were reset to 1 ppb. This percentile-based approach was selected due to the limitations of using a single adjustment to represent the change in the modeled ozone concentrations in moving from the base- to the future-year scenarios. Finally, if either the base-year

[2] The UAM-V *xymap* file contains hourly, gridded, surface-layer ozone concentrations.

or future year percentile concentration was set equal to 1 ppb, the adjustment factor was set equal to 1.

A SAS dataset containing the monitor-level adjustment factors was created for each future-year modeling scenario considered in this study.

Use of Adjustment Factors to Modify Observed Concentrations

Using the calculated adjustment factors for each future-year scenario and the observed monitor- and pseudo-site-level observations, a dataset containing modified observed hourly ozone concentrations for each of the two scenarios was created. Because each monitor has ten adjustment factors per scenario, it was first necessary to rank order the observed concentrations into 10 decile-based groups with ties being assigned to the higher group. Once each of the observed concentrations was identified with a particular decile group, the appropriate adjustment factor was selected and applied:

$$AdjustedConc_i = ObsConc_i * Adj.Factor_{k[ObsConci]}$$

In this equation, {ObsConci} is the set of observed hourly ozone concentrations (in ppm) for a given monitor or pseudo-site. The $k[ObsConc_i]$ is the number of the decile group to which $ObsConc_i$ belongs. $Adj.Factor_{k[ObsConci]}$ is then the appropriate adjustment factor for the decile group to which $ObsConc_i$ belongs. The resulting set of adjusted hourly concentrations, $\{AdjustedConc_i\}$, represents the future-year estimates of the hourly ozone concentrations.

Calculation of Ozone Profiles

Datasets containing the ozone air quality "profiles" were compiled for the base 1990, 2000 Pre-CAAA, 2000 Post-CAAA, 2010 Pre-CAAA, and 2010 Post-CAAA simulations. The profiles used data for the period May through September. The databases contained the number, the arithmetic mean, the median, the (seasonal) second highest, and the 2.5 to 97.5 percentiles (in increments of five) of the hourly concentrations. The profiles are reported at the monitor level and include 842 locations.

The histograms in Figures C-11a through 12b illustrate the distribution of ratios for the 95th percentile monitor-level ozone concentrations corresponding to the 2000 and 2010 simulations, respectively. In this figure, ratios greater than one indicate that the future-year/scenario concentration is greater than the base-year (1990) value, whereas ratios less than one indicate a lower value for the future-year.

The 2000 Pre-CAAA ratios (Figure C-11a) indicate that the 95th percentile ozone concentrations corresponding to this scenario are higher in some areas and lower in other areas than the base-year (1990) values. The ratios generally range from approximately 0.8 to 1.2, but also include some lower values. In contrast, the ratios corresponding to the 2000 Post-CAAA simulation (Figure C-11b) are generally less than one. In this case, the ratios range from approximately 0.75 to 1.1 with only a very small number of values greater than one. There are also some lower values.

Figure C-12a and 12b displays the distribution of ratios of the future-year-scenario to base-year 95th percentile concentrations for 2010. Compared to the histogram plots for 2000, the shift in distribution is such that the ratios are higher for the Pre-CAAA scenario and lower for the Post-CAAA scenario. That is, compared to 2000, concentrations for 2010 are higher relative to the base year under the Pre-CAAA scenario and lower relative to the base year under the Post-CAAA scenario.

For both future years, the ratios indicate that the Post-CAAA concentrations (95th percentile level) are lower than the corresponding Pre-CAAA values (with a few exceptions). This is illustrated in Figures C-13a and C- 13b. The smaller ratios for 2010 (Figure C-13b) reflect the larger differences between the Pre- and Post-CAAA scenarios for this year.

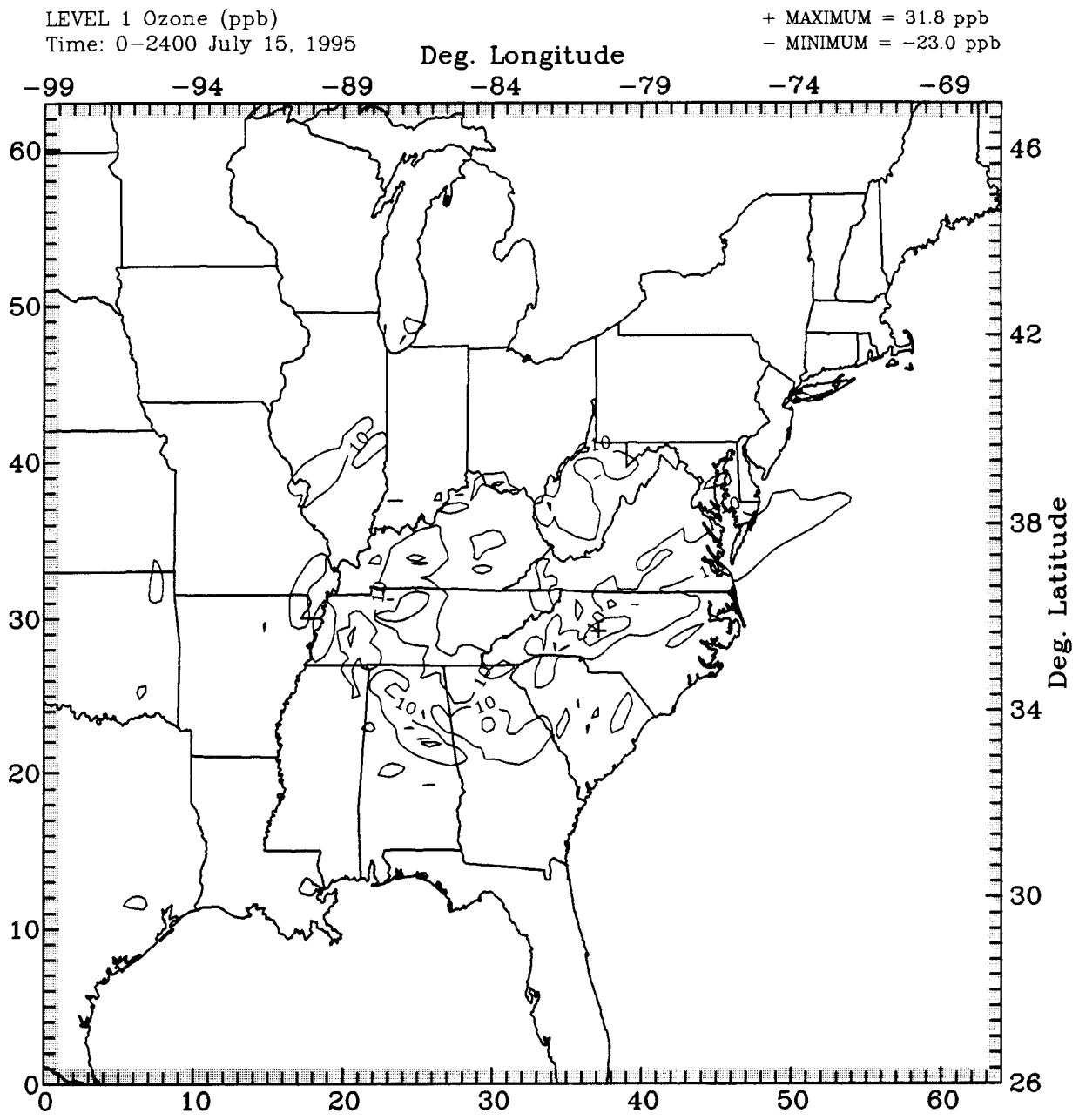


Figure C-2: Difference in daily maximum simulated ozone concentration (ppb) for the 15 July 1995 OTAG episode day: 2010 pre-CAAA90 minus base 1990.

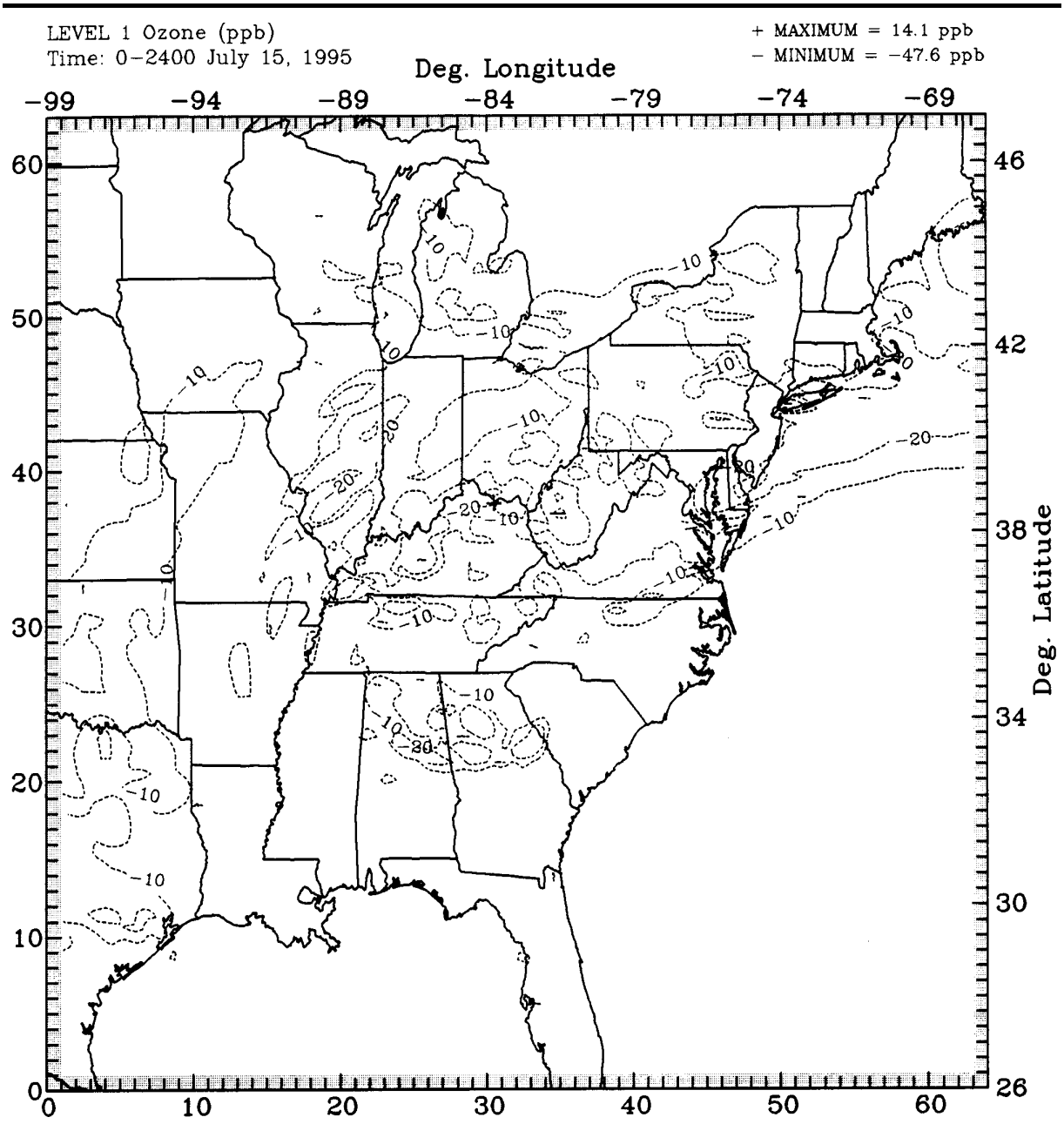


Figure C-3. Difference in daily maximum simulated ozone concentration (ppb) for the 15 July 1995 OTAG episode day: 2010 post-CAAA90 minus base 1990.

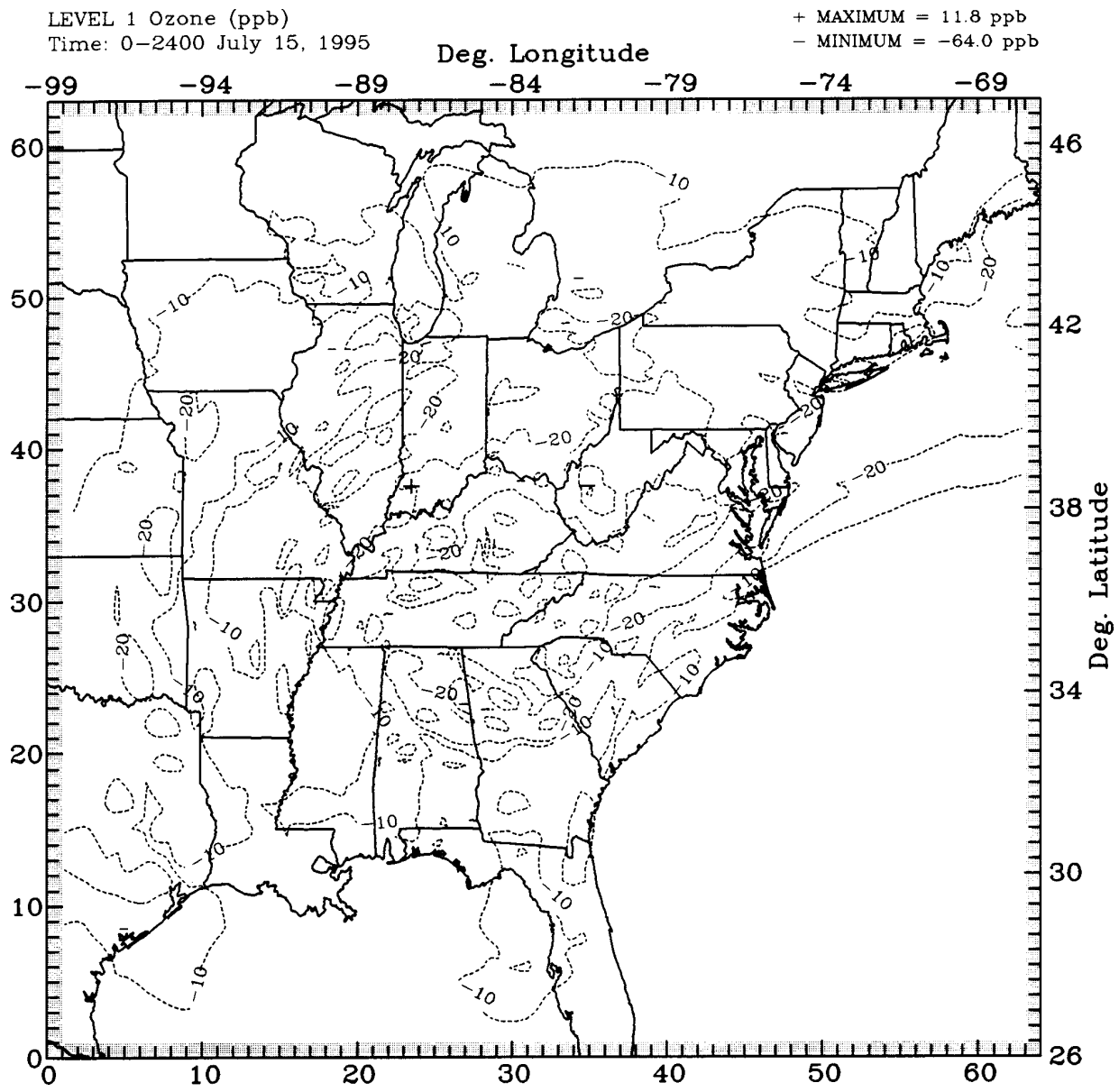


Figure C-4. Difference in daily maximum simulated ozone concentration (ppb) for the 15 July 1995 OTAG episode day: 2010 post-CAAA90 minus pre-CAAA90.

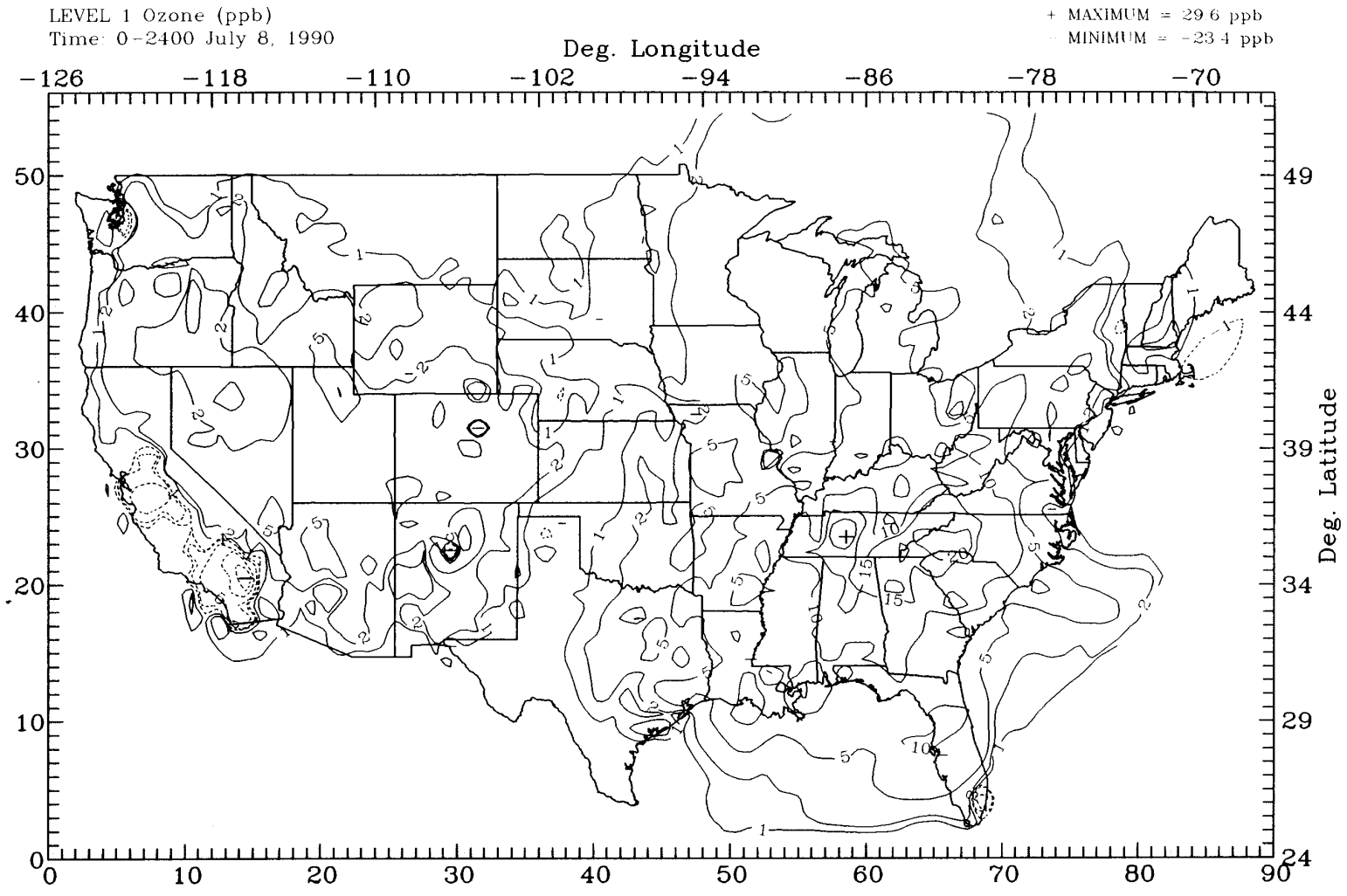


Figure C-5. Difference in daily maximum simulated ozone concentration (ppb) for the 8 July 1990 western U.S. simulation day: 2010 pre-CAAA90 minus base 1990.

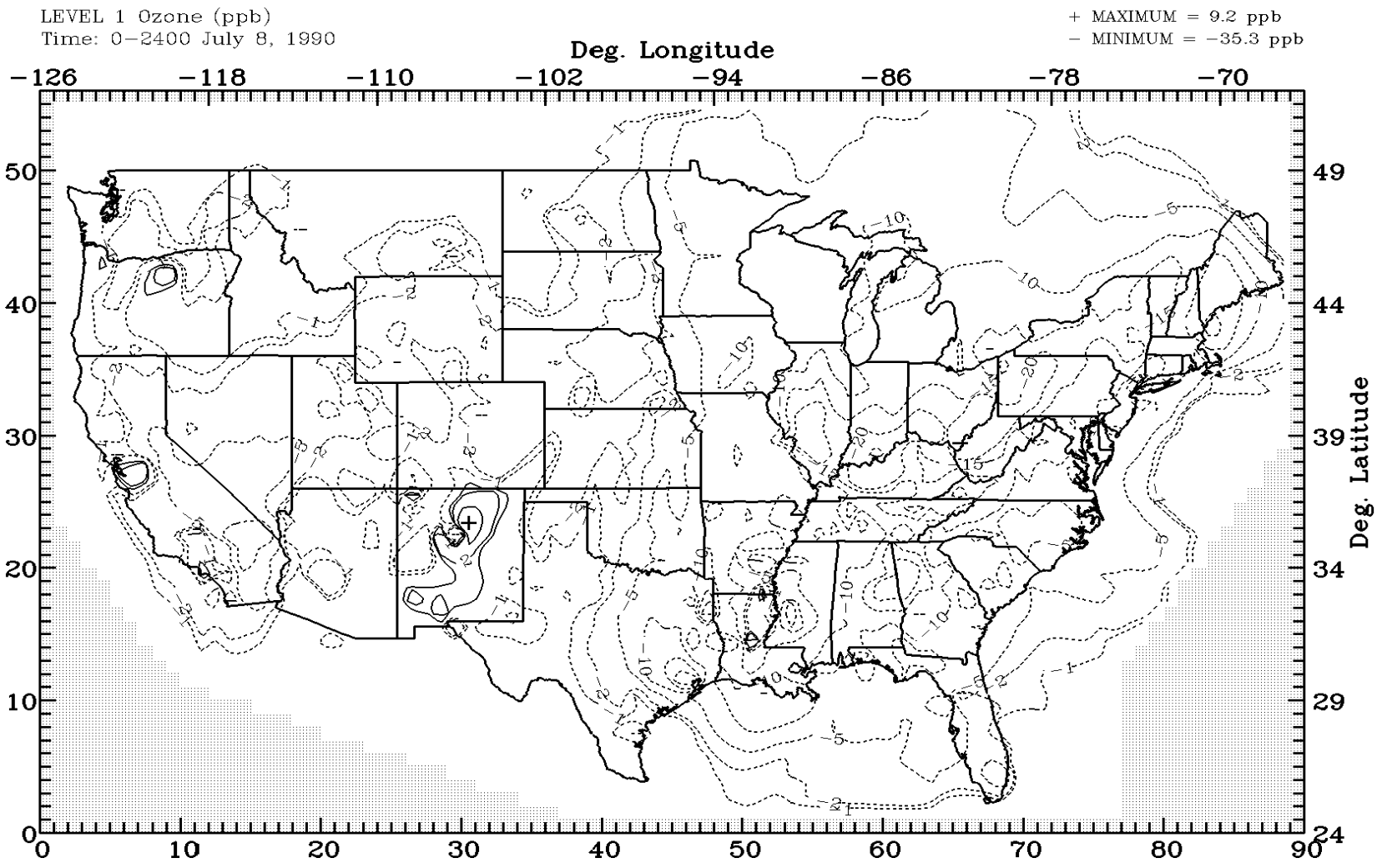


Figure C-6. Difference in daily maximum simulated ozone concentration (ppb) for the 8 July 1990 western U.S. simulation day: 2010 post-CAAA90 minus base 1990.

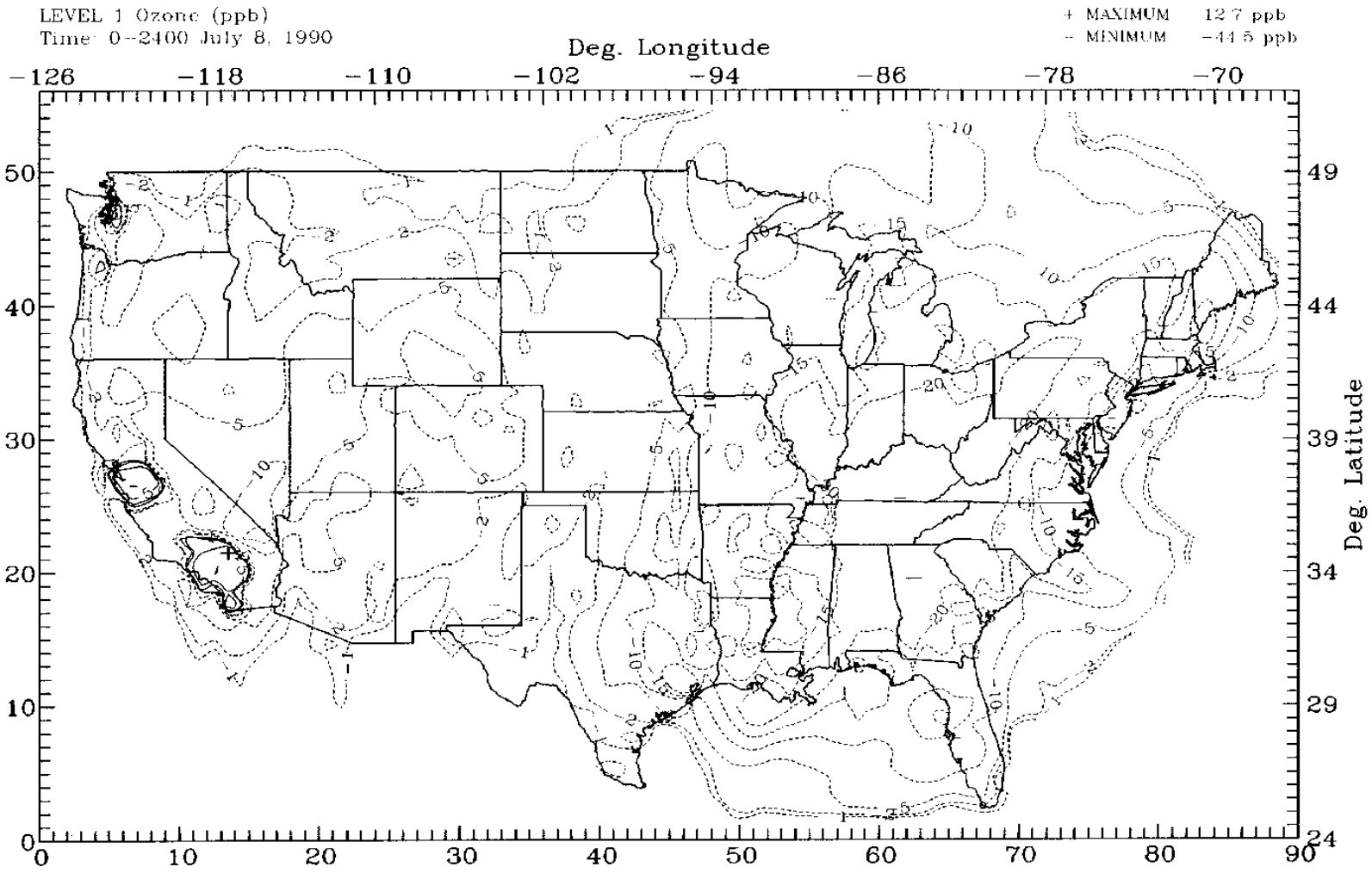


Figure C-7. Difference in daily maximum simulated ozone concentration (ppb) for the 8 July 1990 western U.S. simulation day: 2010 post-CAAA90 minus pre-CAAA90.

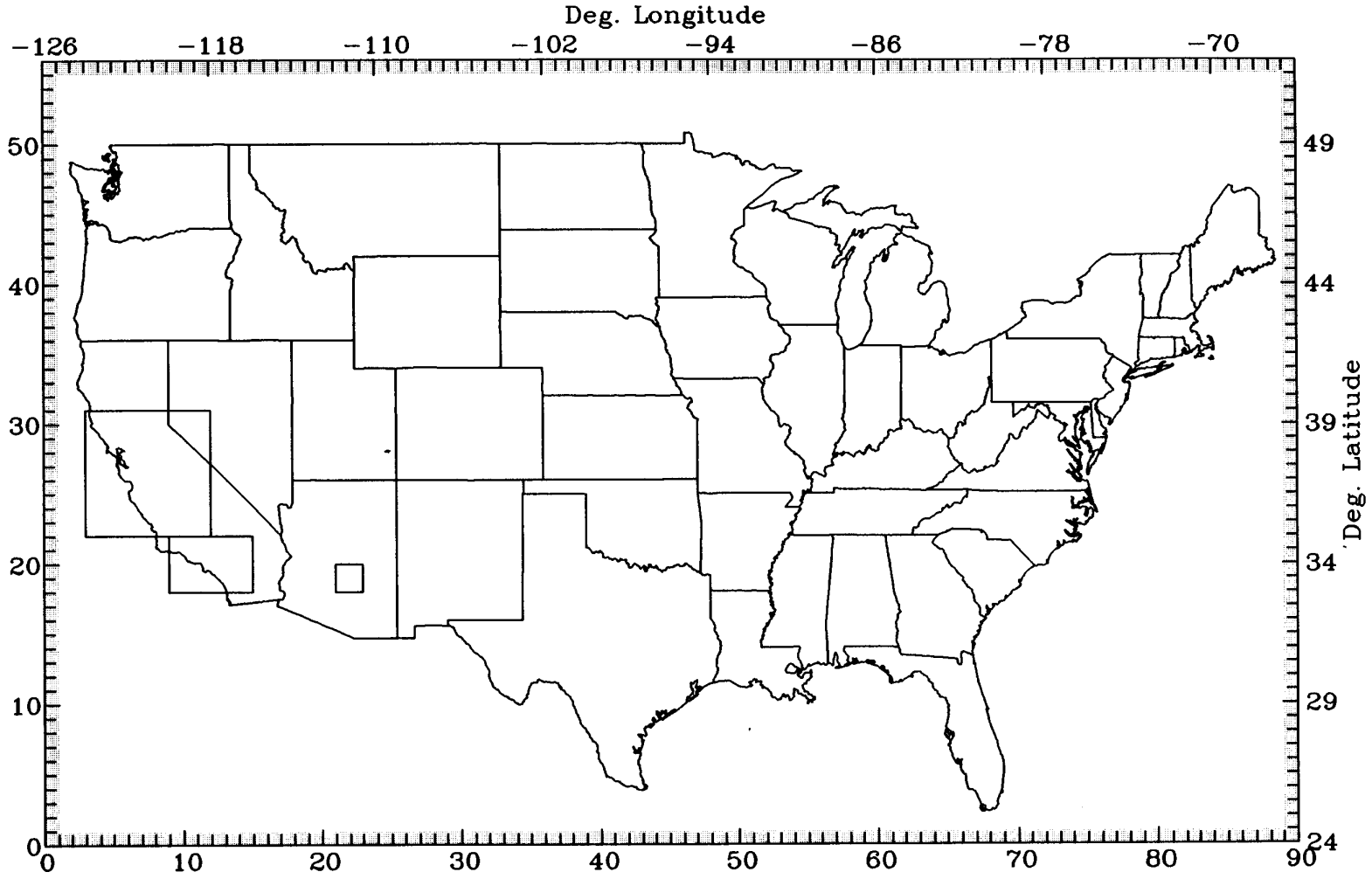


Figure C-8. UAM-V modeling domain for western U.S. analysis with the high-resolution modeling domains for the San Francisco Bay Area, Los Angeles, and Phoenix.

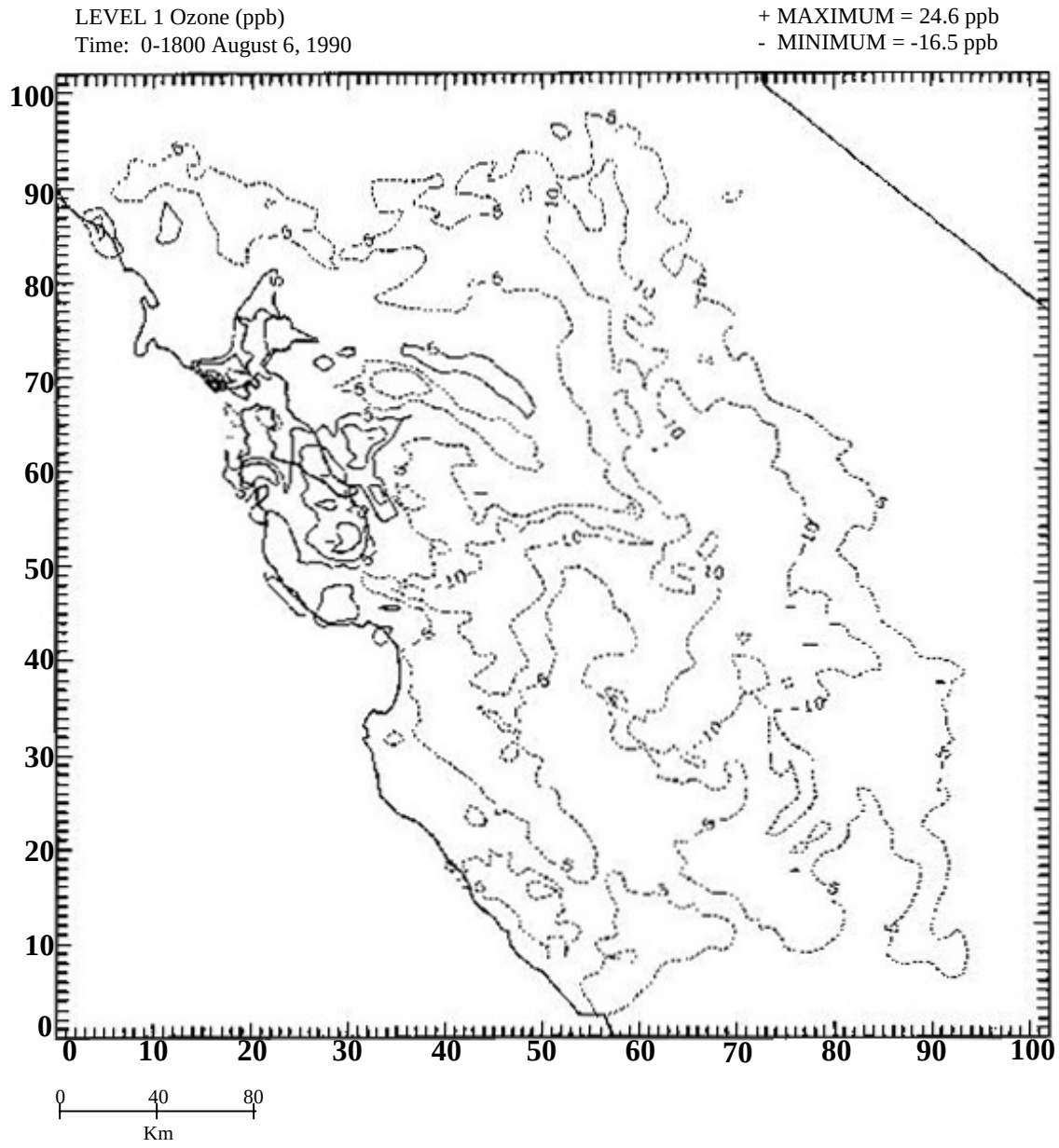


Figure C-9. Differences in daily maximum simulated ozone concentration (ppb) for the 6 August 1990 simulation day for northern California: 2010 post-CAAA90 minus pre-CAAA90.

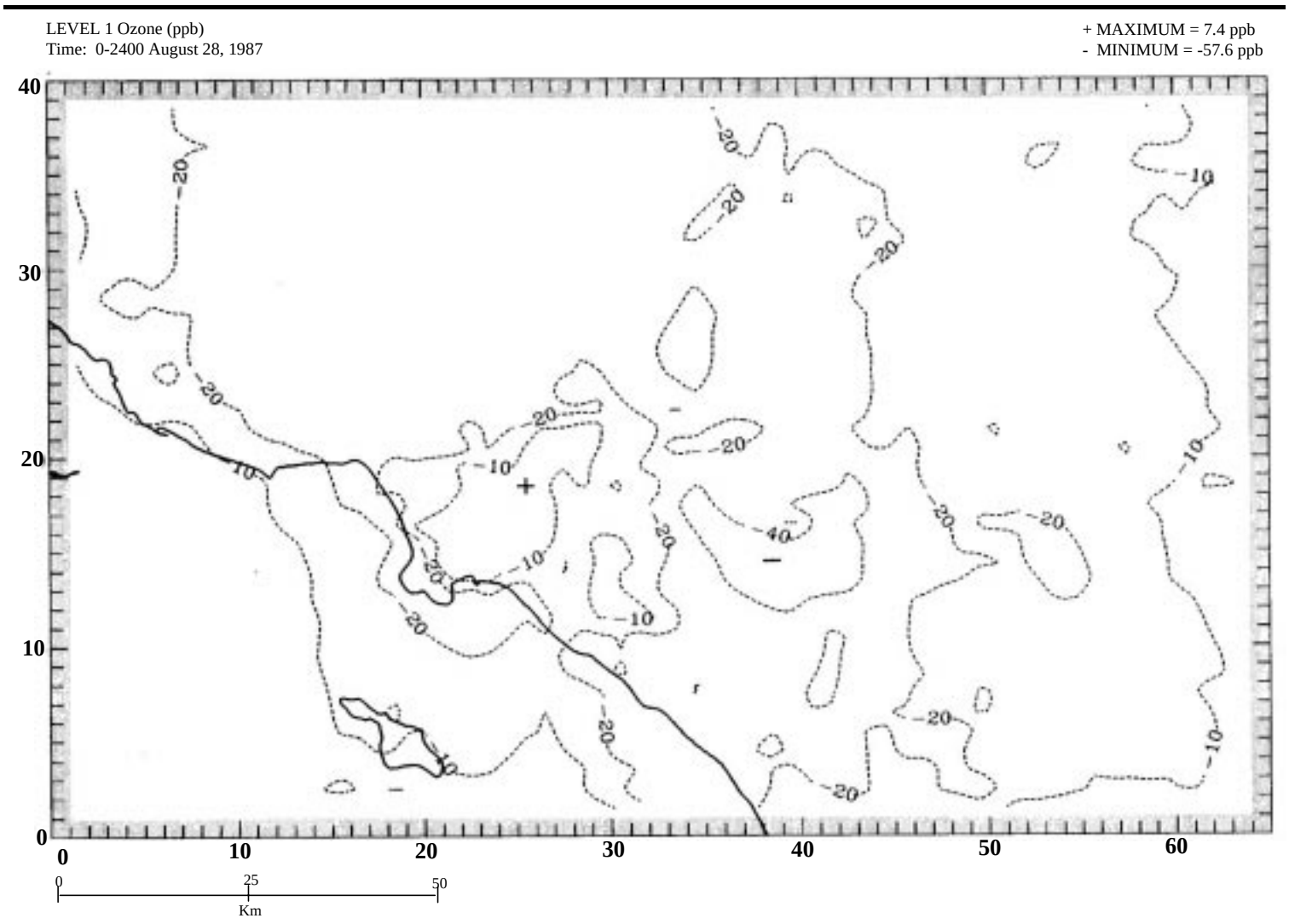


Figure C-10. Difference in daily maximum simulated ozone concentration (ppb) for the 28 July 1987 simulated day for Los Angeles: 2010 post-CAAA90 minus pre-CAAA90.

Figure C-11a. Distribution of Monitor-Level Ratios for 95th Percentiles Ozone Concentration: 2000 Pre-CAAA / 1990 Base-Year

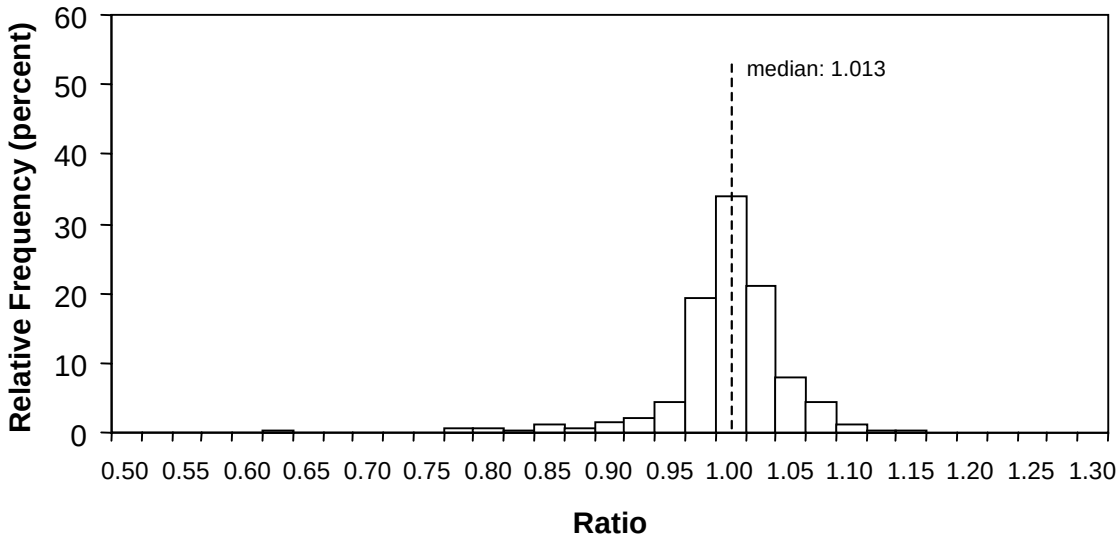


Figure C-11b. Distribution of Monitor-Level Ratios for 95th Percentiles Ozone Concentration: 2000 Post-CAAA / 1990 Base-Year

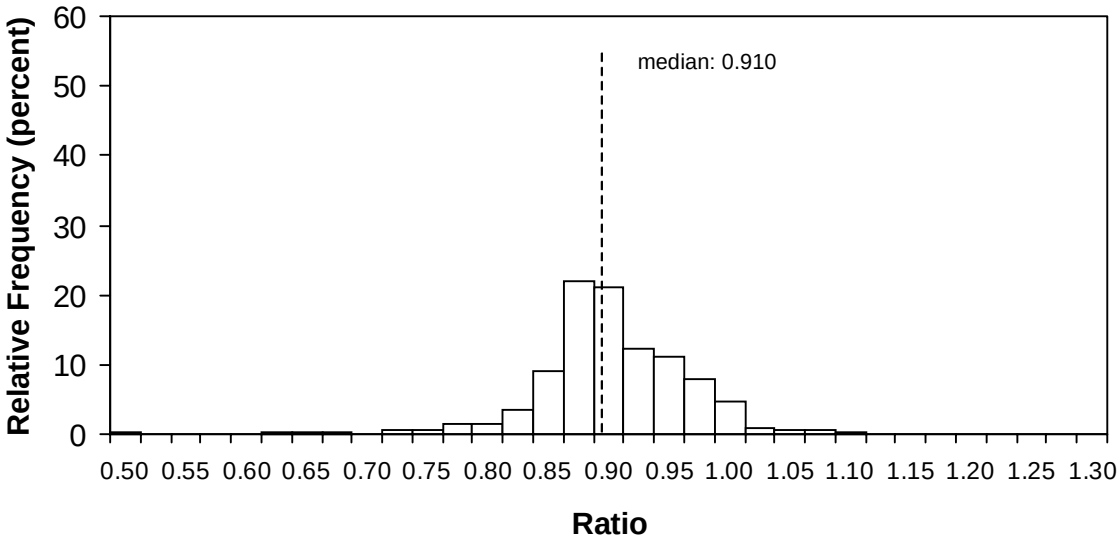


Figure C-12a. Distribution of Monitor-Level Ratios for 95th Percentiles Ozone Concentration: 2010 Pre-CAAA / 1990 Base-Year

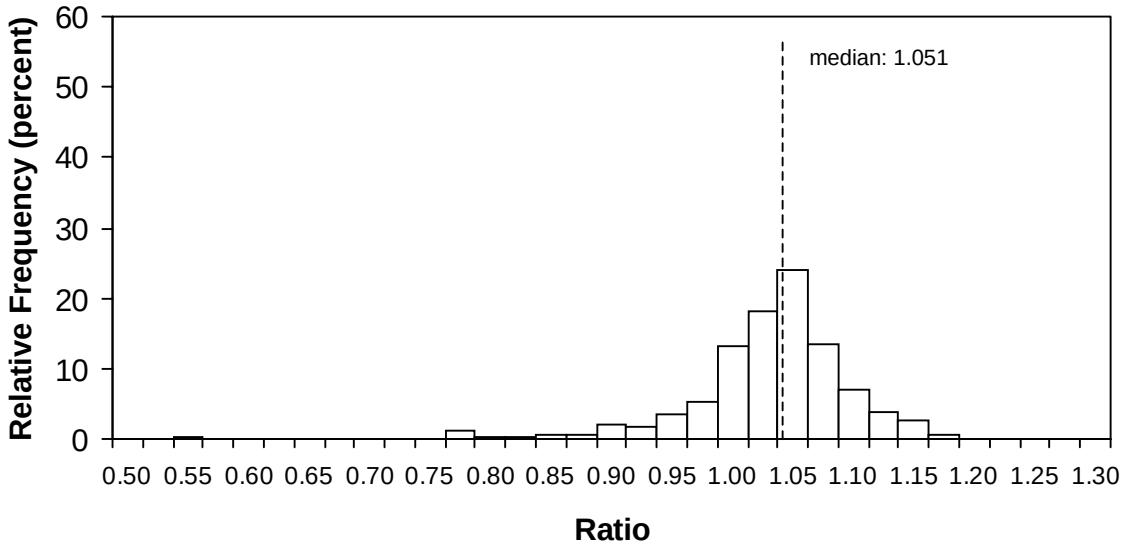


Figure C-12b. Distribution of Monitor-Level Ratios for 95th Percentile Ozone Concentration: 2010 Post-CAAA / 1990 Base-Year

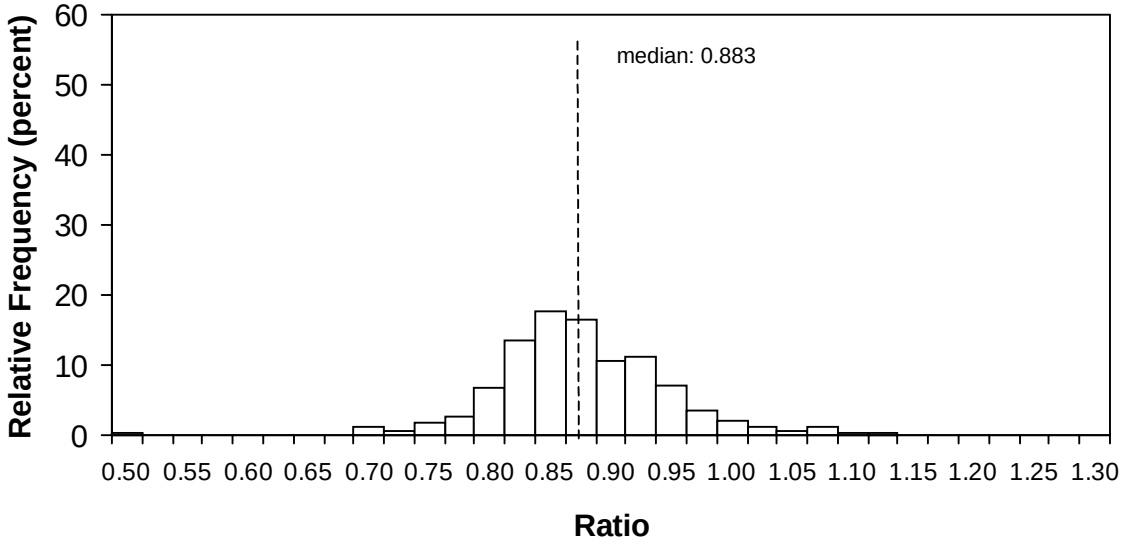


Figure C-13a. Distribution of Monitor-Level Ratios for 95th Percentiles Ozone Concentration: 2000 Post-CAAA / 2000 Pre-CAAA

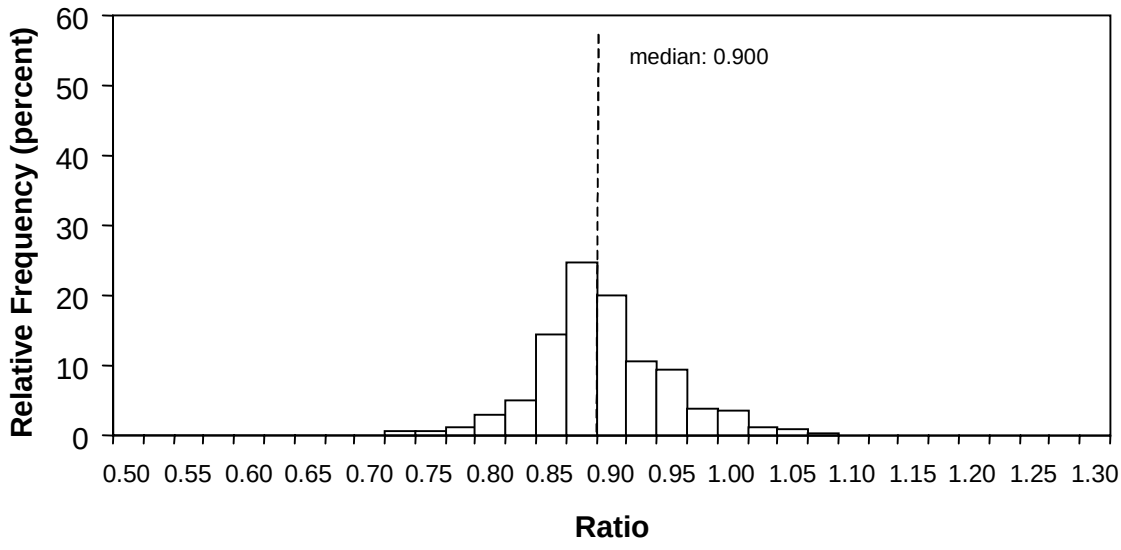
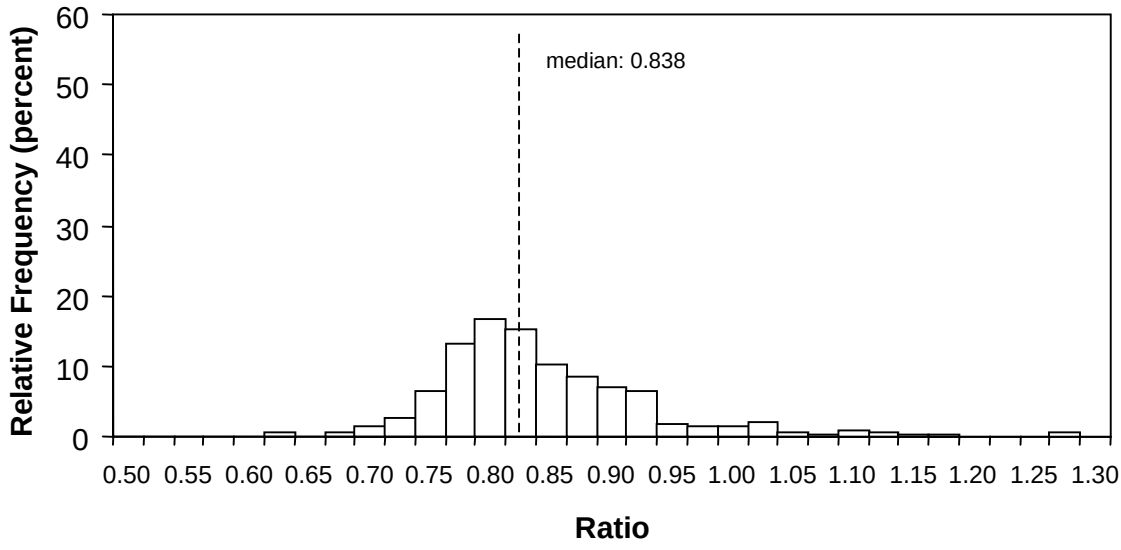


Figure C-13b. Distribution of Monitor-Level Ratios for 95th Percentiles Ozone Concentration: 2010 Post-CAAA / 2010 Pre-CAAA



Estimating the Effects of the CAAA on Particulate Matter

Future-year concentrations of PM_{10} and $PM_{2.5}$ corresponding to the Post-CAAA and Pre-CAAA scenarios were estimated through application of the RADM/RPM and REMSAD modeling systems. The former was used for the eastern U.S., while the latter was applied for the western U.S. Details of both RADM/RPM and REMSAD modeling are presented in this section. Included is an overview of each modeling system, and a description of the application procedures and modeling results. The calculation of PM air quality profiles using the combined modeling results from both models is also described.

For ease of reading, all figures follow the text in this section.

Overview of the RADM/RPM Modeling System

RADM was developed over a ten-year period, 1984-1993, under the auspices of the National Acid Precipitation Assessment Program (NAPAP) to help address policy and technical issues associated with acid deposition. More recently, EPA created the Regional Particulate Model, expanding the Agency's atmospheric modeling capabilities. Functioning together, RADM and RPM help predict PM concentrations by generating estimates of secondary paticulates that comprise a significant portion of total PM.

RADM, a three-dimensional Eulerian grid-based model, is designed to provide a scientific basis for predicting regional air pollution concentrations and levels of acid deposition resulting from changes in precursor emissions. The concentration of a specific pollutant in a grid cell at a specified time is determined by the following factors:

- the emissions rate;
- the transport of that species by wind into and out of the grid in three dimensions;
- movement of the atmosphere via turbulent motion;
- chemical reactions that either produce or deplete the chemical;
- the change in concentration due to vertical transport by clouds;
- aqueous chemical transformation and scavenging; and
- removal by deposition.[3]

RPM is an extension of RADM. Like RADM, RPM is a three-dimensional Eulerian air quality model. Functioning in tandem with RADM, RPM predicts the chemistry, transport, and dynamics of the secondary aerosols of sulfate, nitrate, ammonium, and organics.[4] For this study, however, RPM organic aerosol estimates were not included in the final analysis because the model significantly underestimates organics and the reason for this systematic underestimation has not yet been characterized. The model's predictions of secondary sulfate, nitrate, and ammonium concentrations were used to develop particulate matter concentration estimates.

Application of RADM/RPM for the Eastern U.S.

In this analysis, the RADM/RPM modeling system was used to estimate future year nitrate and sulfate concentrations, two major components of secondary PM. These model results were then used to generate adjustment factors, which in turn aided development of PM predictions for the eastern half of the United States. A summary of the model's application and results follows.

Modeling Domain

The domain of application for both RADM and RPM is eastern North America, from the Rocky

[3]A more detailed description of RADM is provided in R. Dennis, 1995.

[4]A more detailed description of the structure and basic features of RPM is given in F.S. Binkowski and U. Shankar, 1995.

Mountains eastward to Newfoundland, Canada and the Florida Keys. This expansive model area that includes part of Southern Canada allows RADM/RPM to accurately reflect the several-day residence times of sulfur and nitrogen species in the atmosphere and the resulting transport distances of 1,000 kilometers (km) or more that may be covered during that time. The 2,800 by 3,040 km model domain is divided into 80-km grid cells. Nested within this domain are a set of finer resolution 20-km grid cells, covering the geographic region extending eastward from central Illinois to the Atlantic Ocean and southward from Sudbury, Ontario to the upper section of North Carolina (Figure C-14). The model also consists of vertical layers that, in total, stretch 16 km above ground level.

Simulation Periods

RADM/RPM model runs were conducted for 30 five-day periods. The 30 periods, which represent dominant transport regimes spanning four years, were randomly selected to develop annual averages. Later, to develop warm season (May through September) and cold season (October through April) averages, they were divided into these two seasonal groups. Annual warm and cold season averages were developed using a weighting scheme based on the frequency of occurrence of transport regimes. To avoid the influence of the model starting up and adjusting to a new set of conditions associated with each period, only results from the last three days of each period were used to estimate PM levels.

Model Inputs

RADM

Detailed emissions and meteorological data are required to run RADM. The emissions inventory for the model must account for both the timing and location of emissions. Accurate model predictions also depend on a host of meteorological inputs, most notably temperature, wind speed, and wind direction.

Separate emissions inventories were used as input in this analysis for each of the emissions scenarios: 1990 base year, 2000 Pre-CAAA, 2000 Post-CAAA, 2010 Pre-CAAA, and 2010 Post-CAAA.[5] These scenarios and their accompanying inventories, described in more detail in Appendix A, incorporate emissions from all five major source categories: industrial point sources, utilities, nonroad engines/vehicles, motor vehicles, and area sources. This inventory for each scenario contains hourly, day-specific emissions figures for every source category; area and mobile source data are provided at the county level, while utility and industrial point source emissions are given at the source classification code level.

Biogenic emissions were also included in the RADM input. This inventory was developed from version two of EPA's Biogenic Emissions Inventory System (BIES-2). BEIS-2 estimates biogenic emissions based on a variety of factors including biomass and emissions factors.

The meteorological inputs for RADM were derived using output from the Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) mesoscale model (MM4). Using MM4 results, EPA generated essential grid-specific RADM input, including wind flow patterns, temperatures, and water vapor concentrations.

RPM

RPM requires inputs similar to those described for RADM. This model uses a subset of RADM emissions data and the RADM meteorological fields. Additional RPM inputs include atmospheric water data generated by RADM and RADM-predicted levels of oxidants, nitric acid, and ammonia.

[5]See Pechan, June 1998 for a detailed description of the emissions scenarios developed for this analysis.

RADM/RPM Simulation Results

Model Performance

The assessment of model performance for particulate models is a difficult task due to a relative lack of data and information regarding the spatial distribution, composition, and size fractionation of airborne particulates. Development and evaluation of particulate measurement and modeling techniques are active areas of research. As a result, there are currently no standard approaches or model performance criteria for the evaluation of regional-scale particulate models.

Development of RADM began in the mid-1980's. The evolution of this model, along with its application and performance evaluation have all been documented extensively by NAPAP.[6] RADM continues to undergo periodic peer review, evaluations, and improvements.[7] In addition to the present study and the section 812 retrospective analysis, RADM has been used in other Agency studies of acid deposition[8] and in assessments of deposition of nitrogen to coastal estuaries.[9]

RPM was evaluated by comparing the model's 1990 base year seasonal nitrate and sulfate estimates with observed data measured by EPA's Clean Air Act Status and Trends Network (CASTNet). CASTNet is a network of monitors distributed throughout the Eastern U.S. that measures dry deposition of atmospheric sulfur and nitrogen compounds. RPM predictions for particulate sulfate and CASTNet data are provided in Table C-6. Examination of these ambient concentrations shows that RPM predicts the significant seasonal differences in sulfate production, although the model overestimates the annual average sulfate concentration by approximately 20 percent.

Table C-7 displays RPM and CASTNet seasonal average nitrate concentrations and ratios showing the fraction of total nitrate that is in particulate form. Comparison of the values in this table indicate that RPM accurately captures the ratio of particulate to total nitrate, but underestimates overall nitrate levels in the colder months and overestimates them during the warmer months. Averaged over the entire year, however, RPM results and CASTNet data are similar.

Table C-6
Comparison of CASTNet and RPM Average Concentration of SO_4

Season	CASTNet SO_4 ($\mu g/m^3$)	RPM SO_4 ($\mu g/m^3$)
Warm	7.8	9.1
Cold	3.7	3.6
Annual	5.4	6.6

[6]Chang, J. et al. 1987, Chang, J. et al. 1990, and Dennis, R. et al. 1990.

[7]Dennis, R. et al. 1993, McHenry J. and Dennis, R. 1994, and External Review Panel 1994.

[8]U.S. EPA, 1995.

[9]Dennis, R. 1997 and EPA 1997.

Table C-7
Comparison of CASTNet and RPM
Average Concentrations and Fractions of NO_3

Season	CASTNet NO_3 ($\mu g/m^3$)	RPM NO_3 ($\mu g/m^3$)	CASTNet NO_3/t-NO_3 (ratio)	RPM NO_3/t-NO_3 (ratio)
Autumn	1.39	1.25	0.42	0.42
Winter	1.67	1.01	0.44	0.44
Spring	0.85	1.07	0.24	0.24
Summer	0.42	0.57	0.14	0.10
Annual	1.06	1.06	0.31	0.27

RADM/RPM Modeling Results

RADM/RPM generated estimates of nitrate and sulfate concentrations for the years 2000 and 2010 under both the Pre- and Post-CAAA scenarios. These two constituents are major components of secondary PM. As described in more detail later in this appendix, these RADM/RPM results were used to project 1990 observed nitrate and sulfate concentrations to future year levels. From these future year estimates, monitor-level PM_{10} and $PM_{2.5}$ concentrations were calculated for 2000 and 2010.

Comparison of 1990 base year PM levels with future year Pre- and Post-CAAA estimates shows that under the Pre-CAAA scenario, concentrations of PM_{10} and $PM_{2.5}$ are generally expected to increase from base year levels. Under the Post-CAAA scenario, both PM_{10} and $PM_{2.5}$ concentrations are predicted to decrease throughout much of the U.S. in both 2000 and 2010, with greater decreases expected in 2010. The histograms in Figures C-21 through C-24 show the relationship between base year and future year PM estimates. In these figures, ratios greater than one indicate that the future year concentration is greater than the 1990 base year value, while ratios less than one indicate a lower value for the future. Figures C-25 and C-26 show the relationship between Pre- and Post-CAAA PM estimates. All of these histograms present data for the entire U.S., including RADM/RPM data for the East and REMSAD data for the West (see below).

Overview of the REMSAD Modeling System

The Regulatory Modeling System for Aerosols and Deposition (REMSAD) programs have been developed to support a better understanding of the distributions, sources, and removal processes relevant to fine particles and other airborne pollutants, including soluble acidic components and toxics. Consideration of the different processes that affect primary and secondary (i.e., formed by atmospheric processes) particulate matter at the regional scale in different places is fundamental to advancing this understanding and to assessing the effects of proposed pollution control measures. These same control measures will, in most cases, affect ozone, particulate matter and deposition of pollutants to the surface.

The REMSAD system was initially focused on atmospheric aerosols and the deposition of toxic pollutants such as mercury from the air to the surface. Any modeling system for aerosols and deposition must be built on the foundation of an atmospheric transport and dispersion model. Many atmospheric dispersion models have been developed since the late 1970s and applied for various purposes. Urban and regional air quality models are generally based on the Eulerian approach. The REMSAD system is built on the foundation of the UAM-V regional air quality model, which includes a number of advantageous capabilities. The REMSAD aerosol and toxics

deposition module (ATDM) is capable of "nesting" a finer-scale subgrid within a coarser overall grid, which permits high resolution over receptor regions without an intolerable computing burden. The modeling system may thus be applied at scales ranging from a single metropolitan region to a continent containing multiple urban areas.

The REMSAD system consists of a meteorological data preprocessor, the core aerosol and toxic deposition model (ATDM), and postprocessing programs. The ATDM is a three-dimensional grid model designed to calculate the concentrations of both inert and chemically reactive pollutants by simulating the physical and chemical processes in the atmosphere that affect pollutant concentrations. The basis for the model is the atmospheric diffusion or species continuity equation. This equation represents a mass balance in which all of the relevant emissions, transport, diffusion, chemical reactions, and removal processes are expressed in mathematical terms. The model is usually exercised over a multi-day period, typically a full year.

Fine particles (or aerosols) are currently thought to pose one of the greatest problems for human health impacts from air pollution. The major factors that affect aerosol air quality include:

- The spatial and temporal distribution of toxic and particulate emissions including sulfur dioxide (SO_2), oxides of nitrogen (NO_x), volatile organic compounds (VOC), and ammonium (NH_3) (both anthropogenic and nonanthropogenic),
- The size composition of the emitted PM,
- The spatial and temporal variations in the wind fields,
- The dynamics of the boundary layer, including stability and the level of mixing,
- The chemical reactions involving PM, SO_2, NO_x and other important precursor species,
- The diurnal variations of solar insulation and temperature,
- The loss of primary and secondary aerosols and toxics by dry and wet deposition, and
- The ambient air quality immediately upwind and above the region of study.

The ATDM module simulates these processes when it is used to simulate aerosol distribution and toxic deposition. The model solves the species continuity equation using the method of fractional steps, in which the individual terms in the equation are solved separately in the following order: emissions are injected; horizontal advection/diffusion is solved; vertical advection/diffusion and deposition is solved; and chemical transformations are performed for reactive pollutants. The model performs this four-step solution procedure during one half of each advective (driving) time step, and then reverses the order for the following half time step. The maximum advective time step for stability is a function of the grid size and the maximum wind velocity or horizontal diffusion coefficient. Vertical diffusion is solved on fractions of the advective time step to keep their individual numerical schemes stable. A typical driving time step for coarse (50–80 km) grid spacing is 10–15 minutes, whereas time steps for fine grid spacing (10–30 km) are on the order of a few minutes.

Model inputs are prepared for meteorological and emissions data for the simulation days. Once the model results have been evaluated and determined to perform within prescribed levels, a *projected* emission inventory can be used to simulate possible policy-driven emission scenarios.

REMSAD provides gridded averaged surface and multi-layer instantaneous concentrations, and surface deposition output for all species and grids simulated. The averaged surface concentrations and depositions are intended for comparison with measurements and ambient standards. The instantaneous concentration output is primarily used to restart the model, and to examine model results in the upper levels. Concentrations of particulates are passed as input to a module that estimates atmospheric visibility. Wet and dry acidic deposition fluxes are calculated hourly and may be accumulated for any desired interval.

The particulate matter species modeled by REMSAD include a primary coarse fraction

(corresponding to particulates in the 2.5 to 10 micron size range), a primary fine fraction (corresponding to particulates less than 2.5 microns in diameter), and several secondary particulates (e.g., sulfates, nitrates, and organics). The sum of the primary fine fraction and all of the secondaries is taken to be roughly representative of $PM_{2.5}$. Table C-8 lists the simulated species written to the REMSAD output files.

A number of issues are particularly important to a successful application of REMSAD for evaluating the atmospheric transport and deposition of pollutants. These include the meteorology, accuracy and representativeness of the emission inventory, resolution, structure and extent of the modeling grid, and the treatment of urban areas in both the source and receptor areas of the computational grid. Accurate representation of the input meteorological fields is necessary both spatially and temporally in order to adequately capture the complex effects of terrain on airflow and hence transport and deposition of pollutants. In addition the meteorology must be sufficiently resolved in order for the model to accurately diagnose the appropriate cloud characteristics required by the various parameterizations of the cloud processes treated by the model. The required input fields include temporally varying three dimensional gridded wind fields, temperature, humidity and vertical exchange coefficients in addition to the surface pressure and precipitation rates.

Version 4.0 of the REMSAD modeling system (with simplified ozone chemistry) was employed for this study.

Table C-8
REMSAD Output File Species

REMSAD Species[1]	Gas/Aerosol	Description
NO	G	Nitric oxide
NO_2	G	Nitrogen dioxide
SO_2	G	Sulfur dioxide
CO	G	Carbon monoxide
NH_3	G	Ammonia
VOC	G	Volatile organic compounds
HNO_3	G	Nitric acid
PNO_3	A	Particulate nitrate
GSO4	A	Particulate sulfate (gas phase production)
ASO4	A	Particulate sulfate (aqueous phase production)
NH4N	A	Ammonium nitrate
NH4S	A	Ammonium sulfate
SOA	A	Secondary organic aerosols
POA	A	Primary organic aerosols
PEC	A	Primary elemental carbon
Pmfine	A	Primary fine PM (<2.5 microns)
Pmcoarse	A	Primary coarse PM[2] (2.5 to 10 microns)

Sulfate=GSO4+ASO4+NH4S

Nitrate=PNO3+NH4N

Total PM2.5 surrogate=sulfate+nitrate+SOA+POA +Pmfine

[1] These are names used in the model and, for the aerosols, are not necessarily the correct molecular formula (the integers are subscripted only when the formula correctly reflects the species).

[2] Note that (for consistency with the REMSAD User's Guide) we are using the terminology "coarse PM" to mean PM in the size range of 2.5 to 10 microns, which is not in agreement with general use, which defines coarse PM to be particles with size greater than 2.5 microns.

Application of REMSAD for the Western U.S.

For this study, the REMSAD modeling system was applied for the analysis of PM and visibility in western U.S. Although the modeling domain includes the entire U.S. (contiguous 48 states), only the results for the western U.S. were used to calculate the future-year PM concentration profiles. However, the results for the entire domain are presented here. The application procedures and modeling results are summarized in this section.

Modeling Domain

The REMSAD modeling domain encompasses the contiguous 48 states. The domain extends from 126 degrees west longitude to 66 degrees west longitude, and from 24 degrees north latitude to 52 degrees north latitude. A grid cell size of 2/3 longitude by 1/2 latitude (approximately 56 by 56 km) was used across the grid, resulting in a 90 by 55 grid (4,950 cells) for each vertical layer. Eight vertical layers were used for the PM modeling and the first layer results were used to estimate future air quality for the surface monitoring sites. Although REMSAD covers the entire U.S., in this analysis only results for their 11 westernmost states are used.

Simulation Periods

Four simulation periods or episodes were modeled. These episodes correspond to the four seasons of the year and consist of the first ten days of the months of May (spring), July (summer), October (fall), and December (winter).

Model Inputs

The REMSAD modeling system also requires a variety of input files that contain information pertaining to the modeling domain and simulation period. These include gridded, day-specific emissions estimates and meteorological fields; initial and boundary conditions; and land-use information.

Separate emission inventories were prepared for the base-year and each of the future-year scenarios. All other inputs were specified for the base-year model application (1990) and remained unchanged for each future-year modeling scenario.

Modeling Emission Inventories

The data and methodologies used to prepare the REMSAD modeling emission inventories for this study were consistent with those used for the photochemical modeling, but included primary particulates and other species as required for the particulate chemistry. Similar to UAM/UAM-V, REMSAD, requires detailed emission inventories, containing temporally allocated emissions for each grid cell in the modeling domain for each species being simulated. EPS 2.5e was used for the emissions processing. Note that this system has been specifically designed to accommodate regional-scale model applications of particulate matter and toxic species as well as ozone precursors.

The emissions scenarios for this study included 1990 base, 2000 Pre-CAAA, 2000 Post-CAAA, 2010 Pre-CAAA, and 2010 Post-CAAA scenarios. Each inventory includes typical season weekday area source emissions, typical summer or winter day utility emissions (as appropriate), typical season weekday non-utility point source emissions, and typical season day biogenic emissions.

The anthropogenic input emissions inventory data were provided by Pechan (1998). These included area and point source emissions data from the National Particulates Inventory (by county and for specific point sources); county-level vehicle miles traveled (VMT) estimates; mobile-source emission factors for VOC, NO_x, and CO; and PM emission estimates for mobile sources. Note that road dust and other primary particulates are included in the area-source emissions file.

Seasonal biogenic emission estimates for the domain were prepared using version 2 of the EPA's UAM Biogenic Emissions Inventory System (BEIS-2).

BEIS-2 (which estimates biogenic emissions based on various biomass, emission, and environmental factors) utilizes land-use information to determine the distribution of biogenic emissions.

Preliminary processing of the data prior to the application of the EPS 2.5e system was necessary. This consisted of generating the on-road mobile emissions and reformatting all data into AMS and AFS workfile format. Particulate matter pollutants from on-road mobile emissions were provided at county level and were broken down into 12 different urban and rural roadway classifications. To take advantage of the temporal information provided in the utility emissions data, seasonal AFS workfiles were generated separately for the summer and winter months.

All anthropogenic emissions inputs to the various models were preprocessed through the EPS 2.5e system. Point, area, and on-road mobile source emission data were processed separately to facilitate both data tracking for quality control and the use of the data in evaluating the effects of alternative control strategies on simulated air pollutant concentrations. Temporal and spatial allocation were performed as described in Section III.

Primary particulate and secondary particulate precursor emissions are basically derived from particulate matter species, i.e., PM_{10}, $PM_{2.5}$, and NH_3. Therefore a chemical speciation scheme that differs from that for VOC speciation is applied. Table C-9 provides the chemical speciation applied for REMSAD.

Table C-9

Chemical Speciation Schemes Applied for REMSAD

VOC: VOC
NH_3: NH_3
NO_x: NO_X, NO, NO_2
PMC: POA, PEC, GSO_4, PNO_3, PMcoars
PM: POA, PEC, GSO_4, PNO_3, Pmfine

Emission inputs to the REMSAD for selected species, by component, are provided in Table C-10. The purpose of the tables is to quantify the contribution of each source category to total emissions. The species shown include primary particulates and other species that are important to secondary particulate formation. VOC, NO_x, and SO_2 emissions are estimated to increase under the Pre-CAAA scenario and to decrease under the Post-CAAA scenario. For SO_2, the decreases come from the utility sector and are offset by increases in the other components. NH_3 emissions increase for both scenarios and are slightly higher under the Post-CAAA scenario for both years, presumably due to increased use of natural gas fuel. PM_{10} and $PM_{2.5}$ emissions (primary particulates) are similar for all scenarios.

The primary chemical process for PM applications in REMSAD is sulfate formation. In-cloud processes can account for the majority of atmospheric sulfate formation, especially in the wintertime when gas-phase chemistry is slow. The two most important pathways for in-cloud sulfate formation are the reactions of aqueous SO_2 with ozone and hydrogen peroxide (H_2O_2). At cloud pH below 4.5 (most common in the eastern U.S.), the ozone reaction is slow and the H_2O_2 reaction dominates. Since the H_2O_2 is often present at ambient concentrations below those of SO_2, formation of sulfate can be limited by the availability of H_2O_2, and thus can be quite nonlinear. The formation of H_2O_2 is tied to the overall atmospheric photochemical system, and responds to changes in ambient levels of VOC and NO_x. Because of this link, emission changes for VOC and NO_x may have effects on ambient sulfate levels. In short, the emissions of ozone and PM precursors (i.e., NO_x and VOC) will affect the oxidizing capacity of the troposphere which is represented primarily by the concentrations of radicals and hydrogen peroxide, and thus affect the rate of oxidation of the NO_x and SO_2 to nitrate and sulfate.

In REMSAD, there is no relationship between VOC emissions and the production of secondary organic aerosol (SOA).

Table C-10
Emission Totals by Component for each Scenario for the Entire U.S. (tpd)

VOC

	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	33,972	39,154	27,620	43,708	28,575
Onroad Mobile	18,659	16,454	10,683	18,776	8,804
Point	9,503	10,298	8,457	11,606	9,454
Utility	96	85	85	134	137
Total	**62,229**	**65,991**	**46,845**	**74,224**	**46,970**

NOx

	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	13,766	15,659	15,252	17,697	15,794
Onroad Mobile	20,399	20,660	17,421	24,142	14,696
Point	7,964	8,694	5,645	9,803	5,985
Utility	20,188	22,787	11,170	24,808	10,319
Total	**62,316**	**67,800**	**49,487**	**76,450**	**46,793**

SO2

	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	3,517	4,174	4,174	4,811	4,811
Onroad Mobile	1,555	1,730	924	2,109	1,121
Point	12,808	14,620	14,620	16,422	16,422
Utility	43,380	44,261	28,742	48,482	27,016
Total	**61,260**	**64,786**	**48,460**	**71,823**	**49,369**

NH3

	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	10,230	13,189	13,189	15,710	15,710
Onroad Mobile	544	957	957	1,191	1,194
Point	667	742	742	842	1,015
Utility	-	-	91	-	608
Total	**11,441**	**14,888**	**14,979**	**17,744**	**18,527**

PM10

	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	73,221	74,431	72,640	74,532	72,240
Onroad Mobile	972	799	706	814	563
Point	2,549	2,891	2,891	3,252	3,252
Utility	764	691	697	837	758
Total	**77,507**	**78,812**	**76,933**	**79,435**	**76,813**

PM2.5

	Base 1990	2000 Pre-CAAA	2000 Post-CAAA	2010 Pre-CAAA	2010 Post-CAAA
Area	16,717	17,438	17,147	18,174	17,637
Onroad Mobile	797	618	536	640	391
Point	1,625	1,840	1,840	2,066	2,066
Utility	288	247	250	332	305
Total	**19,427**	**20,143**	**19,773**	**21,212**	**20,398**

Air Quality, Meteorological, and Land-Use Inputs

Initial species concentrations and lateral boundary conditions were specified to approximate background concentrations of the species; for the lateral boundaries the concentrations varied (decreased parabolically) with height. The background concentrations are listed in Table C-11.

Table C-11
Background Species Concentration used for REMSAD Initial and Boundary Conditions.

Species	Concentration (ppd)
NO	0.0
NO2	0.1
SO2	0.7
NH3	0.5
VOC	20.0
NHO3	0.01
PNO3	0.01
GSO4	0.1
ASO4	0.0
NH4N	0.01
NH4S	0.1
SOA	1
POA	1
PEC	5
PMFINE	1
PMCOARS	1

Meteorological inputs were derived based on output from the Pennsylvania State University/ National Center for Atmospheric Research (PSU/NCAR) mesoscale model (MM4). Gridded fields of horizontal wind components, temperature, water-vapor concentration, vertical exchange coefficient, precipitation, and pressure were prepared for input to REMSAD. Land-use information was obtained from the USGS database (at 18 km resolution).

REMSAD Simulation Results

Model Performance

The assessment of model performance for particulate models is a difficult task due to a relative lack of data and information regarding the spatial distribution, composition, and size fractionation of airborne particulates. Development and evaluation of particulate measurement and modeling techniques are active areas of research. As a result, there are currently no standard approaches or model performance criteria for the evaluation of regional-scale particulate models. For this study, model performance for REMSAD was examined by comparing the simulated values of selected species with available data. This comparison is intended to provide an indication as to whether the simulated values represent the concentration levels and the range of concentrations indicated by the available observations.

Summaries of model performance were prepared by comparing the simulated values of PM with observed values representing seasonal averages. Comparisons were performed for the entire domain (entire U.S.), the western U.S., and the eastern U.S. Only the western U.S. results are presented here. Data from both the AIRS and IMPROVE PM monitoring networks were included in the evaluation. REMSAD-derived sulfate and nitrate concentrations were also compared to a small number of IMPROVE measurements.

Scatter plots for PM_{10} are provided in Figures C-15 through C-18. For PM_{10}, there is a tendency for underestimation of the seasonal averages in the western U.S., in particular for the fall and winter simulation periods. Similar plots for $PM_{2.5}$, sulfate, and nitrate are available in (SAI, 1999) and show generally good agreement for these species.

These plots indicate that model performance varies throughout the western U.S. and throughout the year. A closer look at the comparison between the simulated and observed values indicates that the agreement is generally better for the IMPROVE sites and that most of the large underestimation occurs for the AIRS sites. The IMPROVE sites tend to be located in rural areas, while the AIRS sites tend to be located in urban areas. There are numerous possible explanations for the differences. One possibility is that one or more components of the urban emissions may not be accurately represented in the inventory. A second possibility is that the grid resolution (approximately 56 km) is not sufficient to resolve the urban-scale processes influencing particulate formation and transport. It is encouraging that generally good agreement is achieved for the limited number of sulfate and nitrate measurements. Overall, the model performance results suggest that the REMSAD modeling system (including the meteorological, air quality, and geographical inputs) provides a reasonable basis for the Section 812 prospective modeling.

REMSAD Modeling Results

The REMSAD simulation results for the Pre- and Post-CAAA scenarios were used in this study to calculate factors for adjustment of observed data and estimation of future-year concentration levels. These were calculated by comparing the simulated concentrations corresponding to each future-year/scenario simulation with those for the base-year simulation (1990). These comparisons indicate that for both future years and both size categories, the Pre-CAAA simulation results are characterized by increases in PM, while the Post-CAAA results show both increases and decreases. Focusing on the western U.S., the increases occur over the larger urban areas and are likely attributable to increases in areas-source emissions of precursors.

While there are increases in primary particulate emissions for some portions of the west, most of the increases are attributable to secondary particles. Isopleth maps for these comparisons are available in (SAI, 1999).

Figures C-19 and C-20 illustrate the differences in seasonal average simulated PM concentration between the Pre- and Post-CAAA simulations for 2010 for the summer period. The differences are calculated as Post-CAAA minus Pre-CAAA, so that negative values indicate lower concentrations for the Post-CAAA scenario. The simulated values for the Post-CAAA scenario are lower than the corresponding Pre-CAAA values for both years. The magnitude and spatial extent of the decreases is greater for 2010 than for 2000 (not shown).

Calculation of PM Air Quality Profiles

The calculation of PM profiles for 2000 and 2010 (for assessment of the effects of the CAAA) include the use of REMSAD results for the western U.S. and RADM/RPM results for the eastern U.S. As for ozone, this was accomplished using an approach that combines observed data and air quality modeling results to estimate the future-year concentrations. While the overall approach is similar to that for ozone (as described in Section III), there are some differences. The future-year air quality profile estimation methodology for PM, as applied to the analysis of the CAAA, is described in this section.

Overview of the Methodology

The methodology for calculation of the adjustment factors differed slightly for the RADM/RPM and REMSAD applications. For RADM/RPM the modeling results were used to calculate adjustment factors for several PM component species; for REMSAD adjustment factors

for PM_{10} and $PM_{2.5}$ were computed directly from the model output. The adjustment factors for each monitoring site were calculated (using the appropriately matched values) for several different concentration levels (i.e., the changes in concentration are dependent upon concentration level). The species concentrations for each monitoring site (estimated using the observations) were then modified using the site-specific (or grid-cell-specific) adjustment factors. For RADM/RPM, PM concentrations were then recalculated using the resulting component values.

For both models, the ratios were calculated on a seasonal basis and were used accordingly to adjust the observed values. Following adjustment of the observed data, statistical quantities, or "profiles", describing the PM distribution for each monitoring site were then calculated.

Description of the Observation Dataset

One of the first tasks in calculating the future-year PM profiles was the creation of a dataset containing the observed concentrations for all monitoring sites located within the modeling domain for the year 1990.

The starting point for this analysis is a database retrieved from the EPA Aerometric Information System (AIRS) of measured ambient concentrations of TSP, PM_{10}, and $PM_{2.5}$ for the year 1990. Due to the limited number of measurements (usually taken once every six days), data for 1989 and 1991 were also used to supplement the 1990 database. Cross-estimation was performed when one of measurements was missing (i.e., PM_{10} or $PM_{2.5}$). The PM component species (that make up secondary PM) were estimated based on a methodology developed by Langstaff and Woolfolk (1995) for the Section 812 retrospective modeling analysis. Size fractionation (PM_{10} fraction of TSP and $PM_{2.5}$ fraction of PM_{10}) and apportionment of secondary PM species relied on a review of previous studies to provide general relationships used to estimate these components of particulate matter. The relationships used for this study depend only on broad geographic region (East, Central, West), time of year (quarter for PM_{10} and season for $PM_{2.5}$), and whether the monitor is located in an urban or rural setting.

The geographical regions used throughout this analysis are presented in Table C-12. In addition to secondary composition fractions, ratios relating $PM_{2.5}$ to PM_{10} were employed. The literature review conducted for establishing secondary particulate matter concentrations for the 1990 data and the sources of ratios and apportionment factors used in the equations below is discussed in some detail by Langstaff and Woofolk (1995).

It should be noted that there is considerable variability in the size and species composition of particulate matter, not only between different locations, but also from day to day in the same location. The average size fractions and speciation factors used for this study represent a rather sweeping simplification of the actual physical phenomena that are being modeled. However, this may be justified in the context of this study, due to data limitations and the fact that the results are aggregated to the annual level.

As mentioned earlier, cross-estimation of TSP, PM_{10}, and $PM_{2.5}$ was used to estimate values not present in the original AIRS database. The results of a linear regression of TSP versus PM_{10} by region, quarter, and land-use were used to fill in either PM_{10} or TSP, if the other was missing. After this, the results of a linear regression of $PM_{2.5}$ versus PM_{10} by region, season, and land use were then used to fill in $PM_{2.5}$ values where missing. With both estimated and observed TSP, PM_{10}, and $PM_{2.5}$, the coarse PM concentration was calculated as well as the PM concentration greater than 10 microns.

$$PM_{>10} = TSP - PM_{10} \quad (1)$$

$$PM_{C} = PM_{10} - PM_{2.5} \quad (2)$$

Table C-12
Geographical Regions of the U.S.

Central	East	West
Oklahoma	Indiana	Nevada
Missouri	Kentucky	Utah
Kansas	Ohio	Colorado
Nebraska	Michigan	New Mexico
Iowa	Virginia	Arizona
South Dakota	West Virginia	Texas
North Dakota	Pennsylvania	California
Minnesota	New York	Oregon
Wisconsin	Maryland	Washington
Illinois	New Jersey	Idaho
	Connecticut	Wyoming
	Rhode Island	Montana
	Massachusetts	
	Vermont	
	New Hampshire	
	Maine	
	Delaware	
	Washington, DC	
	Florida	
	Georgia	
	Alabama	
	Mississippi	
	Louisiana	
	Arkansas	
	Tennessee	
	North Carolina	
	South Carolina	

$PM_{2.5}$ and coarse PM were partitioned into secondary particulate concentrations. As shown below, each equation illustrates how the secondary particulate concentrations are calculated from coarse and fine PM.

$$S = [PM_{2.5} * r_{s\,2.5}] + [PM_C * r_{s\,C}] \quad (3)$$

$$N = [PM_{2.5} * r_{n\,2.5}] + [PM_C * r_{n\,C}] \quad (4)$$

$$O = [PM_{2.5} * r_{o\,2.5}] + [PM_C * r_{o\,C}] \quad (5)$$

$$P = [PM_{2.5} * r_{p\,2.5}] + [PM_C * r_{p\,C}] \quad (6)$$

where

S = sulfate concentration
N = nitrate concentration
O = organic concentration
P = other particulate concentration
$PM_{2.5}$ = PM less than or equal to 2.5 microns in size
PM_C = PM between 2.5 and 10 microns in size (coarse PM)
$r_{x\,2.5}$ = ratio of <=2.5 micron sulfate (x=s), nitrate (x=n), organic (x=o), and other particulate (x=P) to $PM_{2.5}$
$r_{x\,C}$ = ratio of 2.5-10 micron sulfate (x=s), nitrate (x=n), organic (x=o), and other particulate (x=P) to coarse PM

Note that r_{xx} was based on a review of available data/literature and depends on geographic region,

time of year, and land-use characteristics of the monitoring site location.

The observed and estimated species concentrations were then input into a single AMP350-format datafile. From the information contained in this file, two SAS datasets were created: a concentration dataset and a monitor information dataset. The concentration dataset contains the daily concentrations for each monitor, with each record in the dataset representing a single monitor-day. The monitor information dataset contains monitor-specific information such as land-use and location.

Because PM monitors are typically operated on a one-in-six day monitoring schedule, calculating percentiles for the PM profiles using data for a single year can be very sensitive to the method used in the percentile calculation. This is especially true when a monitor record only needs to be 50 percent complete (i.e., contain at least 30 values) for a profile to be generated. To minimize dependence on the form of the percentile equation, the 1990 PM data were supplemented with that from the years 1989 and 1991. In using multiple years worth of monitoring data, it was discovered that the identifier (ID) corresponding to a monitor in a given physical location could change from one year to the next. Also, a monitor could have moved to a nearby location and been assigned a different ID. It was also possible that the monitor ID for a PM_{10} monitor might be different from that of a TSP or $PM_{2.5}$ monitor despite the fact that their physical separation is zero. Because much of the profile work is dependent upon the monitor ID, this led to a vast increase in the reported number of operating monitors.

To accommodate these possibilities, monitors with different monitor ID's were considered the same monitor if their physical separation was less than or equal to 1 km. Monitoring data from the two monitors were combined. If data existed for both of the monitors on the same day, the daily data from the monitor with the higher ID was removed.

For particulate data, a monitor record was considered to be complete if data were available for 50 percent of the 24-hour observations for a given year (assuming a one-in-six day monitoring schedule). Although three years worth of data were used for the PM analysis, these data were considered to represent one year with respect to the completeness requirement. There were 2048 PM monitors with complete data.

Calculation of Percentile-Based Adjustment Factors

For each future-year modeling scenario, grid-cell-species-season-specific adjustment factors were calculated using the speciated, daily-simulated concentrations from RADM/RPM and REMSAD. Because the species and seasons differed between the two models, the exact calculation of adjustment factors also differed. Nevertheless, the overall approach was the same. Individual monitoring sites were mapped onto the gridded output (to determine the grid cell in which each monitor was located) and the concentrations for the corresponding grid cells were used to calculate a set of adjustment factors for each species, season, and future-year modeling scenario. The adjustment factors were specified to be the ratio of the percentile concentrations for the future- and base-year simulations of a given species-season, where the percentile concentrations were calculated using data for the selected species and season concentrations:

$$\text{Adjustment Factor}_{i,species,season} = \frac{\text{xth Percentile Concentration}_{future\ year,species,season}}{\text{xth Percentile Concentration}_{base\ year,species,season}}$$

$$\{x_i\} = \{10, 30, 50, 70, 90\}$$

For calculation of the percentile concentrations, the empirical distribution function with averaging was employed. Because the concentrations for the lower percentiles can be rather small, a threshold value of 0.01 microgram/m^3 was set to keep the adjustment factors reasonable. In other words, all concentrations below 0.01 microgram/m^3 were reset to 0.01

microgram/m^3. If either the base year or the future ear percentile concentration was set to the minimum value, the adjustment factor was set equal to one. This percentile-based approach was selected due to the limitations of using a single adjustment to represent the change in the modeled PM species concentrations in moving from the base- to the future-year scenarios.

For RADM, adjustment factors were calculated for the sum of sulfate, nitrate, and ammonium. These were calculated for the entire year (i.e., only one "season"). For REMSAD, the adjustment factors were calculated for PM_{10} and $PM_{2.5}$. These were calculated on a seasonal basis.

A SAS dataset containing the monitor-level adjustment factors was created for each future-year modeling scenario considered in this study for this year.

Use of Adjustment Factors to Modify Observed Concentrations

Using the calculated adjustment factors for each future-year scenario and the monitor-level observations, a dataset containing modified PM_{10} and $PM_{2.5}$ concentrations for each of the four future-year scenarios was created. Because each monitor has five adjustment factors per scenario, species, and season, it was first necessary to rank order the observed concentrations into five quintile-based groups (with ties being assigned to the higher group) with respect to the species and season definitions mentioned previously. Thus for RADM, the quintiles were calculated for the daily sum of the observed sulfate, nitrate, and ammonium concentrations over the entire year (ignoring that the data are actually for the years 1989, 1990, and 1991). For REMSAD the quintiles were calculated for the observed daily PM_{10} and $PM_{2.5}$ over each of the four seasons. Once each of the observed concentrations was identified with a particular quintile group, the appropriate adjustment factor was selected and applied to calculate the future-year-scenario PM_{10} and $PM_{2.5}$.

For RADM, the adjustment factor was applied using the following equations:

$$AdjNitrateSulfate_i = ObsNitrateSulfate_i * Adj.Factor_{k[ObsNitrateSulfatei],NitrateSulfate}$$
$$AdjOrganics_i = ObsOrganics_i * 1$$
$$AdjP_i = ObsP_i * 1$$

For example in the first equation, $\{ObsNitrateSulfate_i\}$ is the set of observed daily sums of the nitrate and sulfate concentrations (in micrograms/m^3) for a given monitor. The $k[ObsNitrateSulfate_i]$ subscript is the number of the quintile group to which $ObsNitrateSulfate_i$ belongs. $Adj.Factor_{k[ObsNitrateSulfatei],NitrateSulfate}$ is then the appropriate adjustment factor for $ObsNitrateSulfate_i$. The resulting set of adjusted daily sums of nitrate and sulfate concentrations, $\{AdjNitrateSulfate_i\}$, represents the future year estimates of the daily sum of nitrate and sulfate concentrations. In this case, *P* represents other particulate components. For those monitors within the RADM domain, PM_{10} and $PM_{2.5}$ concentrations were calculated by summing each of the above components.

For monitors within the REMSAD domain, the procedure for calculating the future-year PM_{10} and $PM_{2.5}$ is more direct. Future-year concentrations of these two PM species are calculated using the observed/estimated PM_{10} and $PM_{2.5}$ concentrations and the appropriate adjustment factors:

$$AdjPM10_i = ObsPM10_i * Adj.Factor_{k[ObsPM10i],PM10,season}$$
$$AdjPM2.5_i = ObsPM2.5_i * Adj.Factor_{k[ObsPM2.5i],PM2.5,season}$$

In the first equation, $\{ObsPM10_i\}$ is the set of observed daily PM_{10} concentrations (in micrograms/m^3) for a given monitor. The $k[ObsPM10_i]$ subscript is the number of the quintile group (based on season) to which $ObsPM10_i$ belongs. $Adj.Factor_{k[ObsPM10i],PM10,season}$ is then the appropriate adjustment factor for $ObsPM10_i$. The resulting set of PM_{10} and $PM_{2.5}$ concentrations, $\{ObsPM10_i\}$ and $\{ObsPM2.5_i\}$, therefore represents the future-year estimates of these PM species.

Calculation of PM Profiles

PM_{10} and $PM_{2.5}$ air quality profile databases were compiled for all simulations performed as part of the Section 812 prospective analysis. For each of the particulate species, these data bases contained the number, the arithmetic mean, the median, the annual second highest, and the 2.5 to 97.5 percentiles (in increments of five) of the daily (as available) concentrations. The profiles are reported at the monitor level and include 2048 site locations.

The histograms in Figures C-21a through C-24b illustrate the distribution of ratios for the annual average monitor-level PM_{10} and $PM_{2.5}$ concentrations corresponding to the 2000 and 2010 simulations. In these figures, ratios greater than one indicate that the future-year/scenario concentration is greater than the base-year (1990) value, whereas ratios less than one indicate a lower value for the future-year.

The 2000 Pre-CAAA ratios for PM_{10} (Figure C-21a) indicate that the annual average PM_{10} concentrations corresponding to this scenario are higher in some areas and lower in other areas than the base-year (1990) values. The ratios generally range from approximately 0.95 to 1.1, but also include some higher values. In contrast, the ratios corresponding to the 2000 Post-CAAA simulation (Figure C-21b) are generally less than or equal to one, with most sites being assigned a ratio consistent with a small decrease in annual average PM_{10} concentration. There are also some lower values.

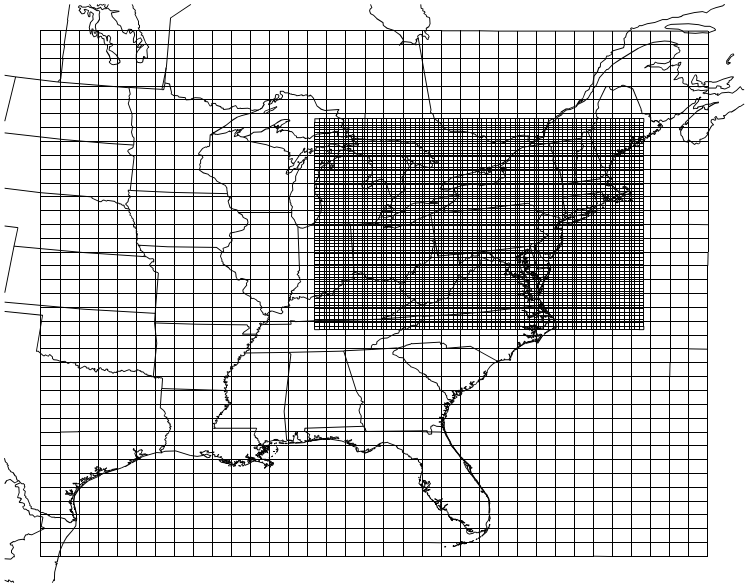
Figure C-22a and C-22b display the distribution of ratios of the future-year-scenario to base-year annual average PM_{10} concentrations for 2010. Compared to the histogram plots for 2000, the ratios are higher for the Pre-CAAA scenario but similar for the Post-CAAA scenario. There is some indication that, by 2010, increases due to growth are limiting the effectiveness of the CAAA measures.

The 2000 Pre-CAAA ratios for $PM_{2.5}$ (Figure C-23a) indicate that the annual average $PM_{2.5}$ concentrations corresponding to this scenario are generally higher than (or equal to) the base-year (1990) values. The ratios generally range from approximately 0.975 to 1.15. In contrast, the ratios corresponding to the 2000 Post-CAAA simulation (Figure C-23b) are generally less than one. In this case, the ratios range from approximately 0.925 to 1.075.

For 2010, the $PM_{2.5}$ ratios (Figures C-24a and C-24b), indicate increases for the Pre-CAAA scenario and mostly decreases for the Post-CAAA scenario. Again, compared to 2000, concentrations for 2010 are higher relative to the base year under the Pre-CAAA scenario and similar to or slightly lower relative to the base year under the Post-CAAA scenario.

For both future years (2000 and 2010), the ratios indicate that the Post-CAAA concentrations (annual average) are lower than the corresponding Pre-CAAA values. This is illustrated in Figures C-25a through C-26b. The smaller ratios for 2010 reflect larger differences between the Pre- and Post-CAAA scenarios.

Figure C-14
80-km RADM Domain



Note: Nested 20-km grid estimates were not used to generate final results, but were used in evaluating the reasonableness of results.

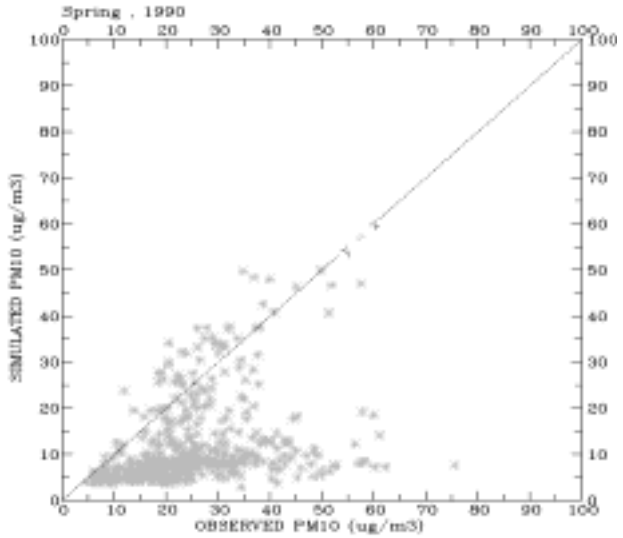


Figure C-15. Comparison of simulated and observed seasonal PM10 concentration (ug/m3) for REMSAD for the western U.S.: spring 1990

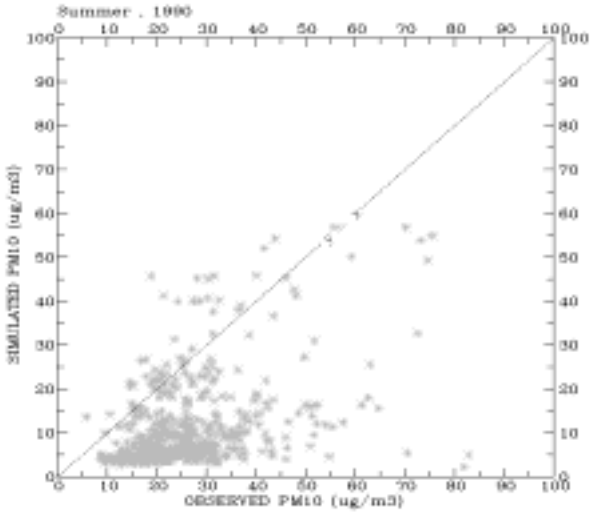


Figure C-16. Comparison of simulated and observed seasonal PM10 concentration (ug/m3) for REMSAD for the western U.S.: summer 1990

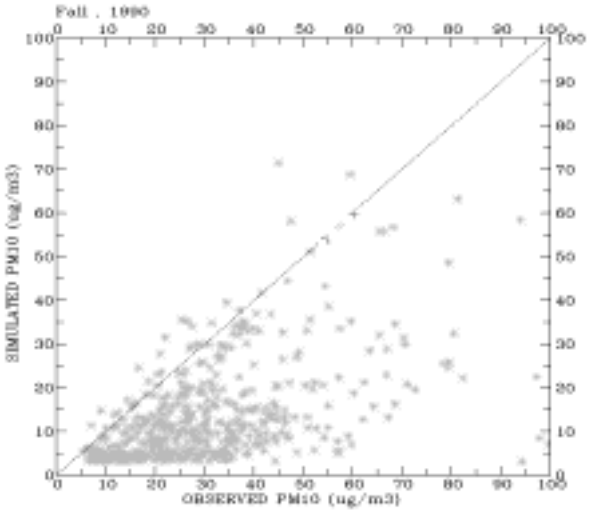


Figure C-17. Comparison of simulated and observed seasonal PM10 concentration (ug/m3) for REMSAD for the western U.S.: fall 1990

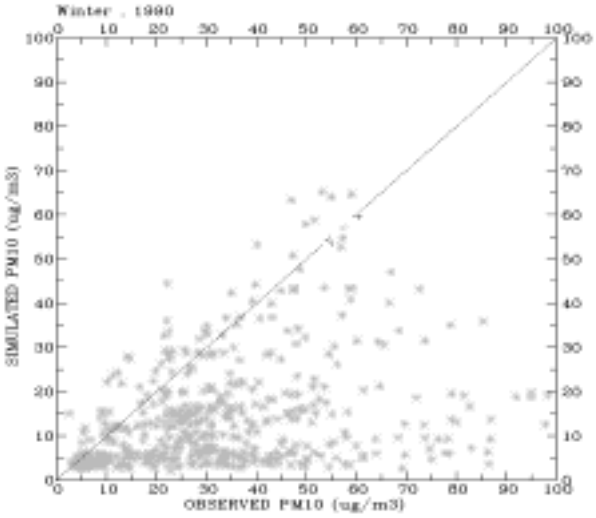


Figure C-18. Comparison of simulated and observed seasonal PM10 concentration (ug/m3) for REMSAD for the western U.S.: winter 1990

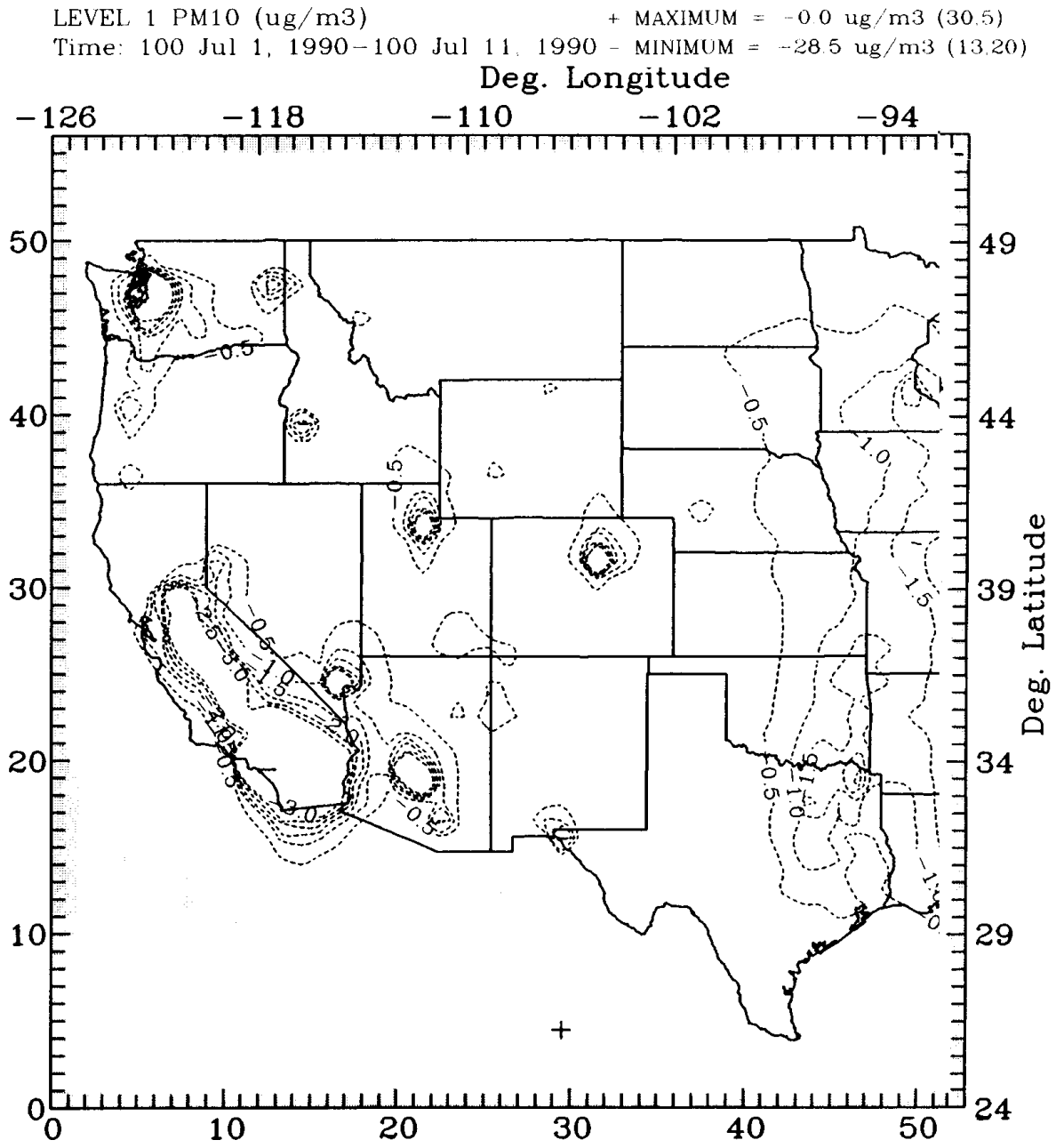


Figure C-19. Difference in seasonal average PM10 concentration (ug/m3) for the summer REMSAD simulation period (1-10 July 1990) for 2010: post-CAAA90 minus pre-CAAA90

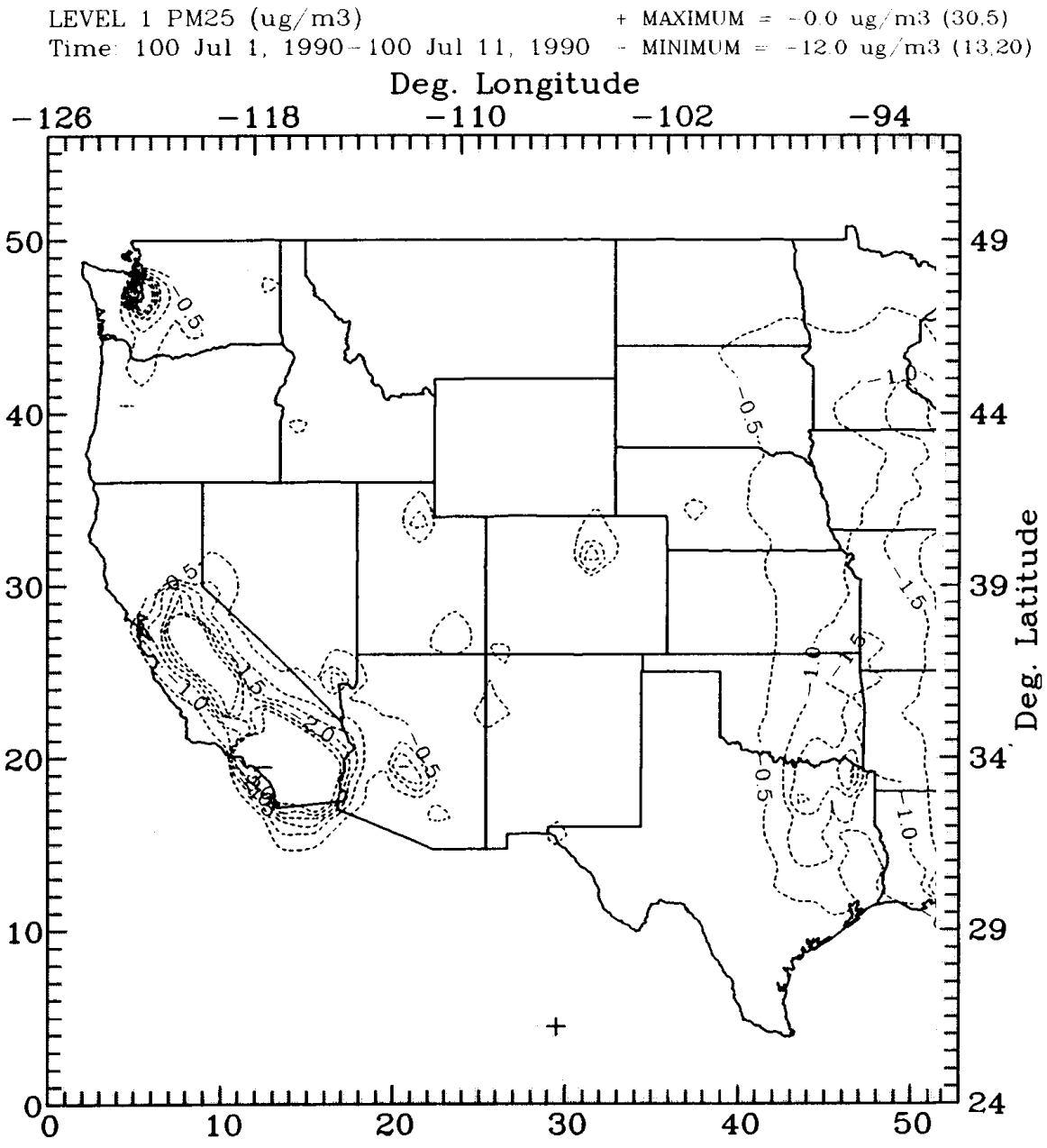


Figure C-20. Difference in seasonal average PM25 concentration (ug/m3) for the summer REMSAD simulation period (1-10 July 1990) for 2010: post-CAAA90 minus pre-CAAA90

Figure C-21a. Distribution of Combined RADM/RPM- and REMSAD-Derived Monitor-Level Ratios for Annual Average PM_{10} Concentration: 2000 Pre-CAAA / 1990 Base-Year

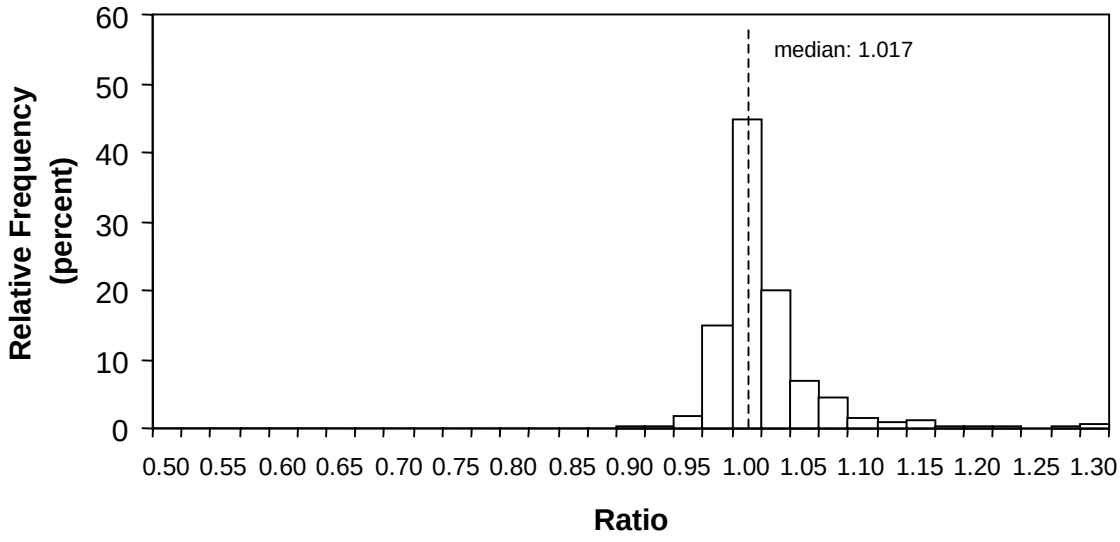


Figure C-21b. Distribution of Combined RADM/RPM- and REMSAD-Derived Monitor-Level Ratios for Annual Average PM_{10} Concentration: 2000 Post-CAAA / 1990 Base-Year

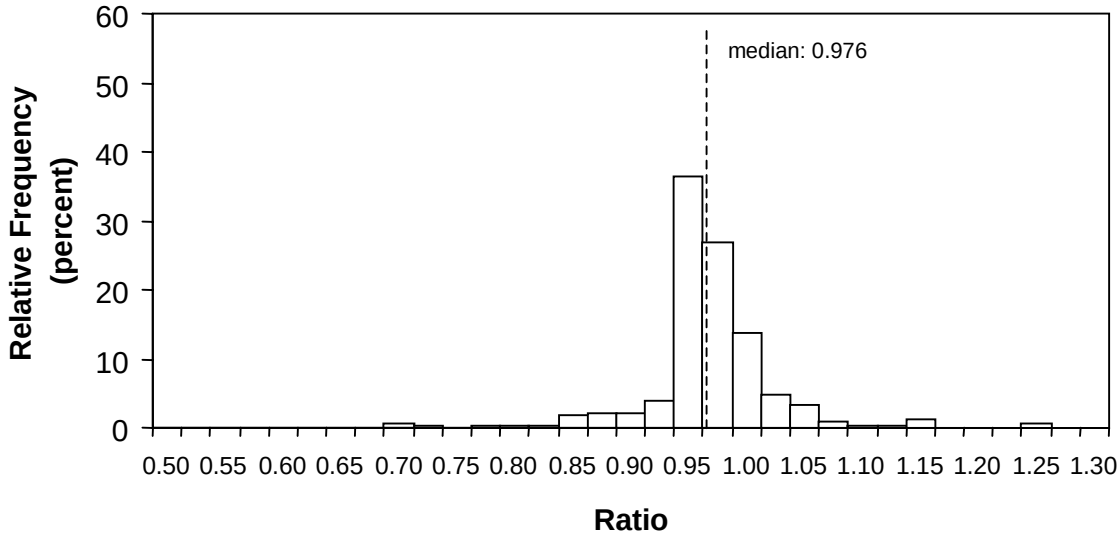


Figure C-22a. Distribution of Combined RADM/RPM- and REMSAD-Derived Monitor-Level Ratios for Annual Average PM_{10} Concentration: 2010 Pre-CAAA / 1990 Base-Year

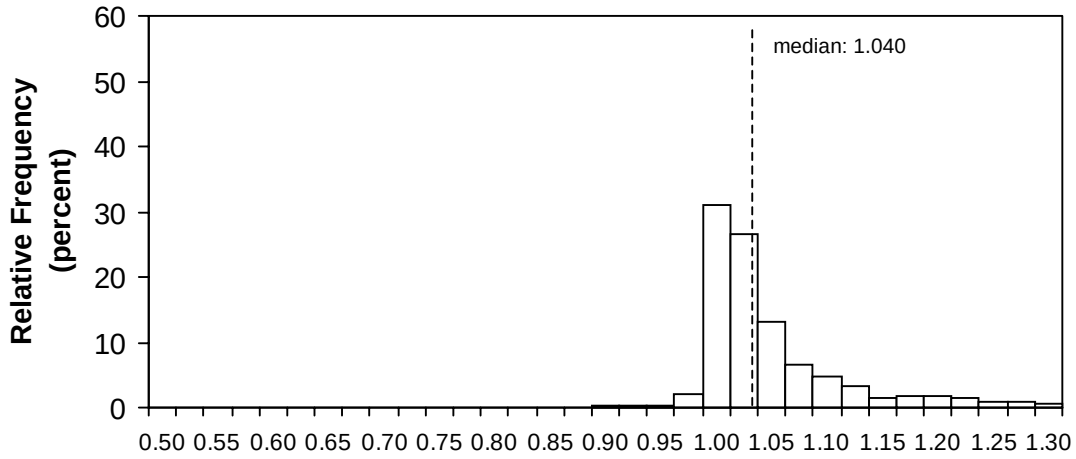


Figure C-22b. Distribution of Combined RADM/RPM- and REMSAD-Derived Monitor-Level Ratios for Annual Average PM_{10} Concentration: 2010 Post-CAAA / 1990 Base-Year

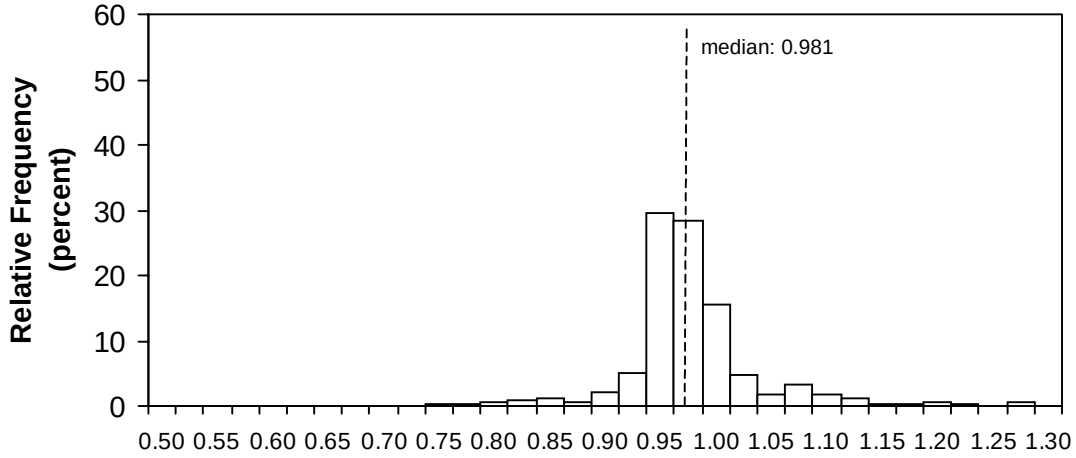


Figure C-23a. Distribution of Combined RADM/RPM- and REMSAD-Derived Monitor-Level Ratios for Annual Average $PM_{2.5}$ Concentration: 2000 Pre-CAAA / 1990 Base-Year

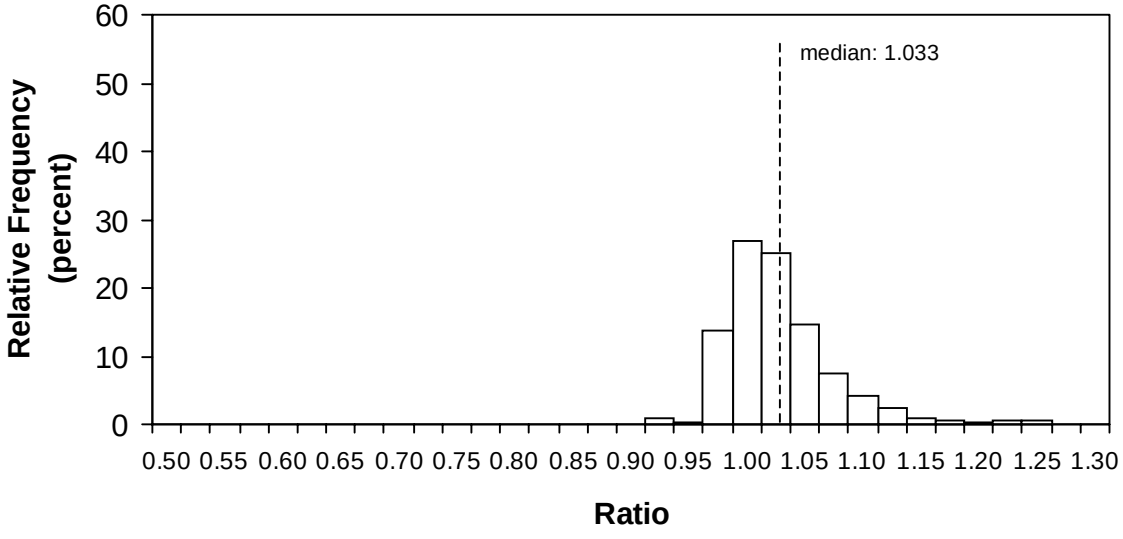


Figure C-23b. Distribution of Combined RADM/RPM- and REMSAD-Derived Monitor-Level Ratios for Annual Average $PM_{2.5}$ Concentration: 2000 Post-CAAA / 1990 Base-Year

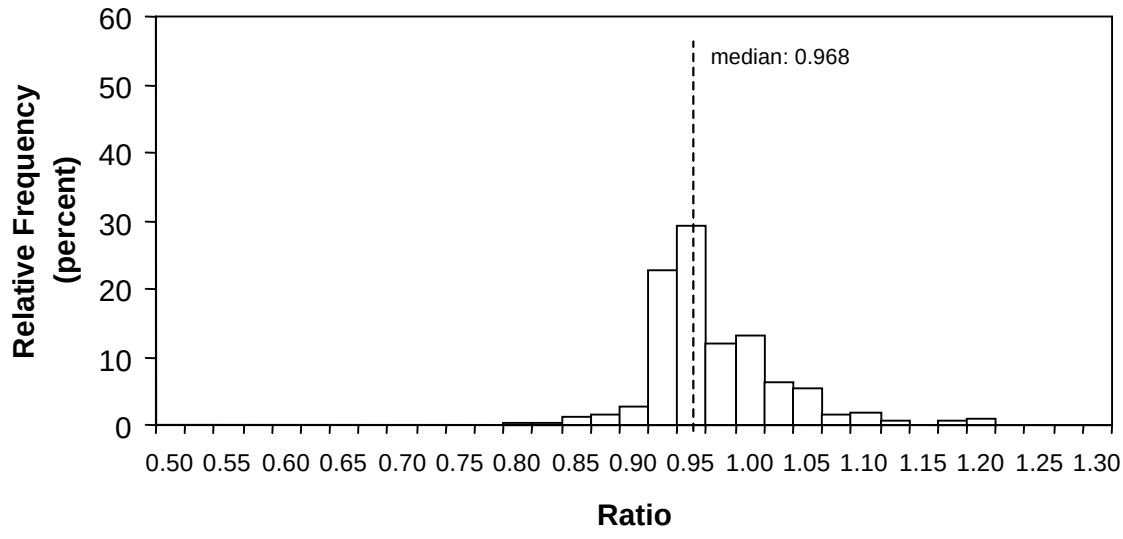


Figure C-24a. Distribution of Combined RADM/RPM- and REMSAD-Derived Monitor-Level Ratios for Annual Average $PM_{2.5}$ Concentration: 2010 Pre-CAAA / 1990 Base-Year

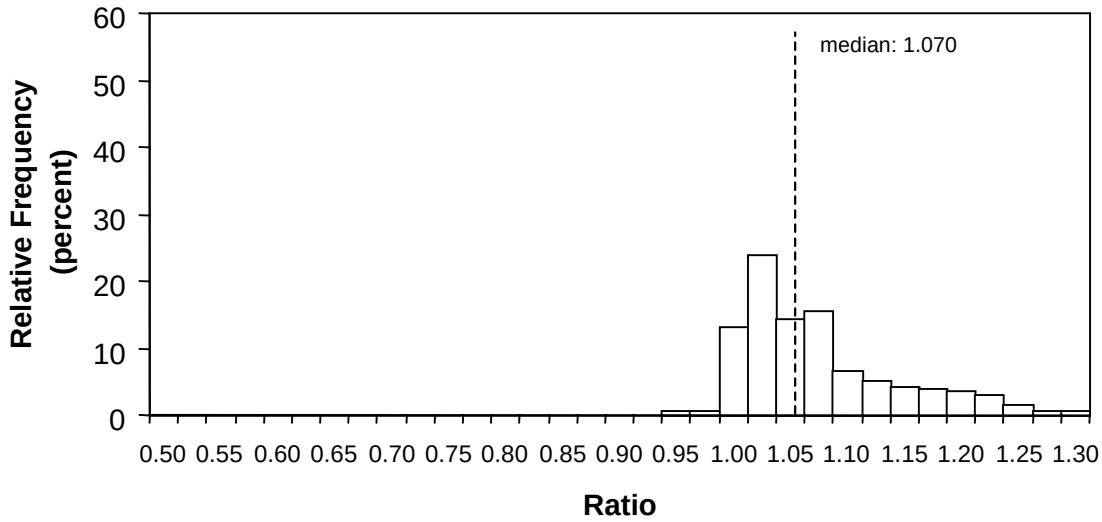


Figure C-24b. Distribution of Combined RADM/RPM- and REMSAD-Derived Monitor-Level Ratios for Annual Average $PM_{2.5}$ Concentration: 2010 Post-CAAA / 1990 Base-Year

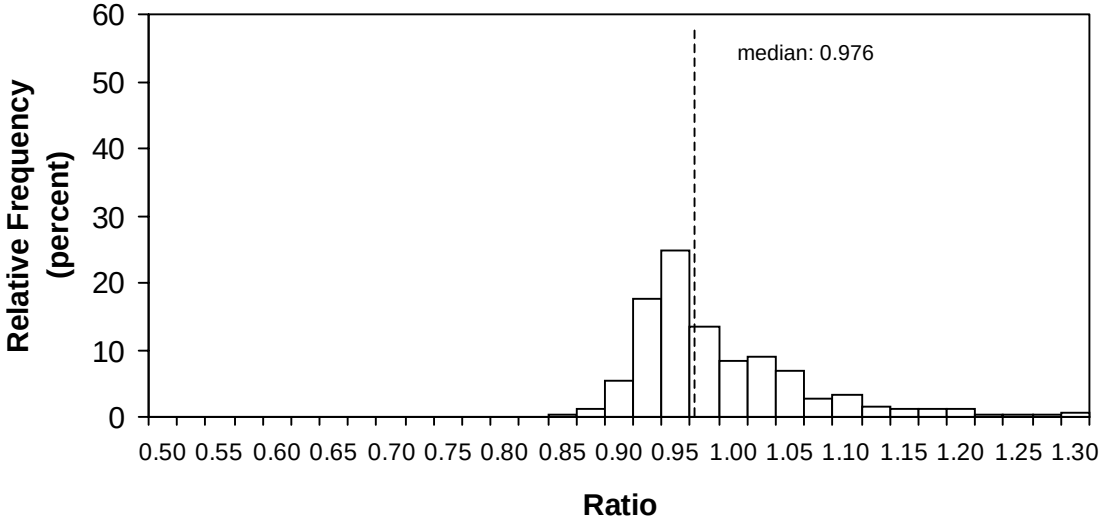


Figure C-25a. Distribution of Combined RADM/RPM- and REMSAD-Derived Monitor-Level Ratios for Annual Average PM_{10} Concentration: 2000 Post-CAAA / 2000 Pre-CAAA

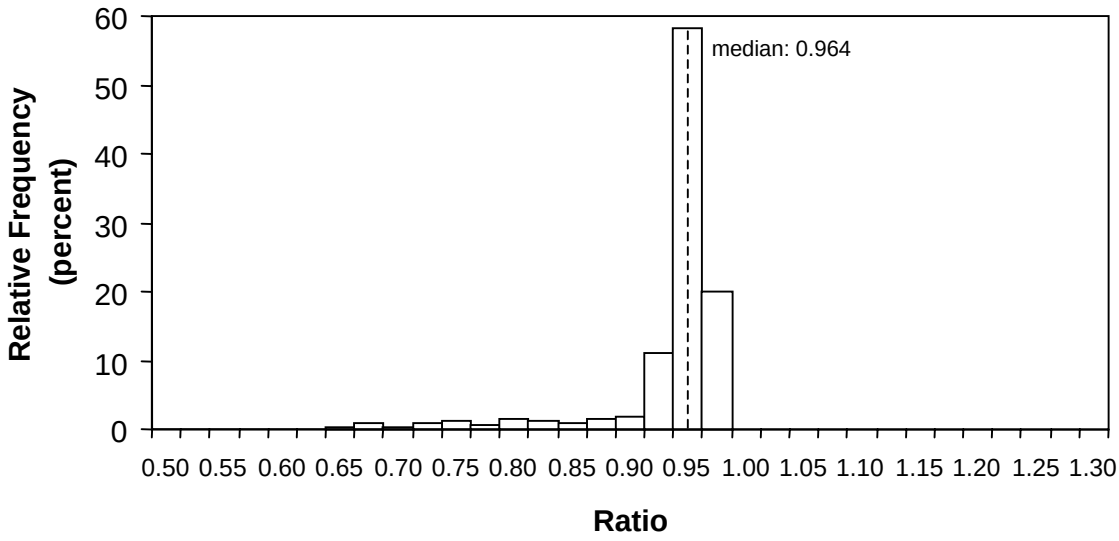


Figure C-25b. Distribution of Combined RADM/RPM- and REMSAD-Derived Monitor-Level Ratios for Annual Average PM_{10} Concentration: 2010 Post-CAAA / 2010 Pre-CAAA

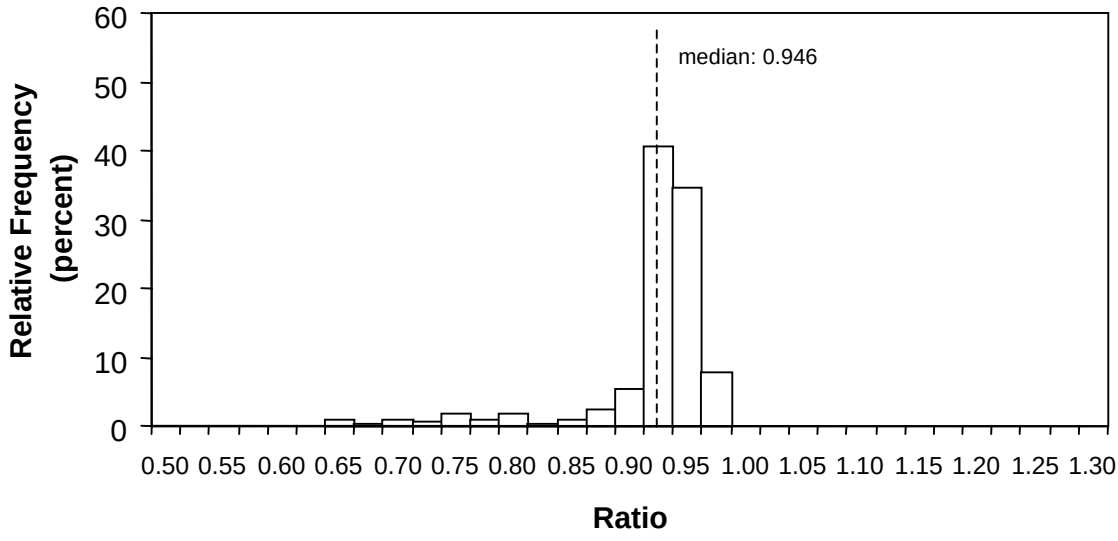


Figure C-26a. Distribution of Combined RADM/RPM- and REMSAD-Derived Monitor-Level Ratios for Annual Average $PM_{2.5}$ Concentration: 2000 Post-CAAA / 2000 Pre-CAAA

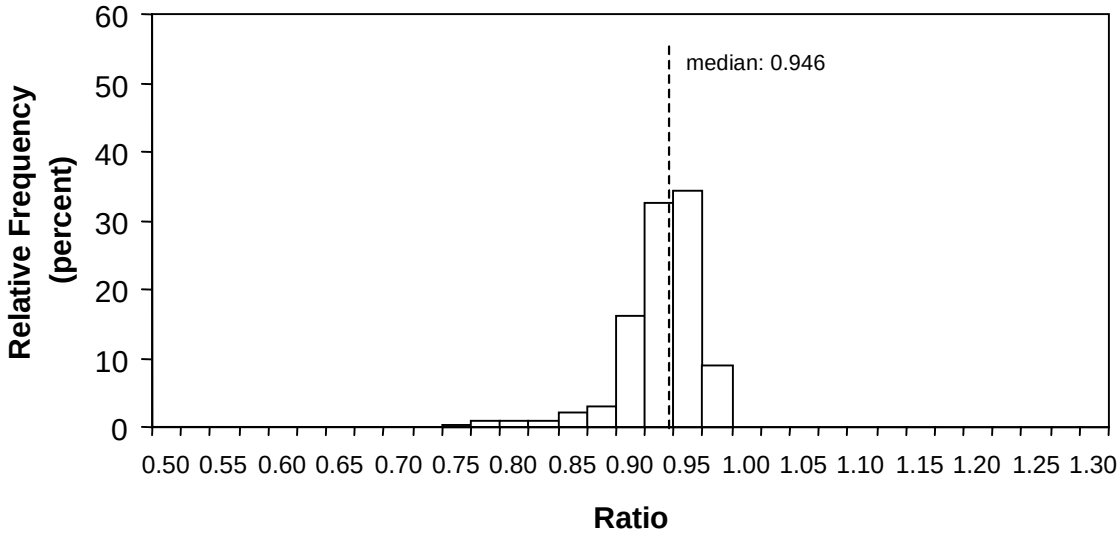
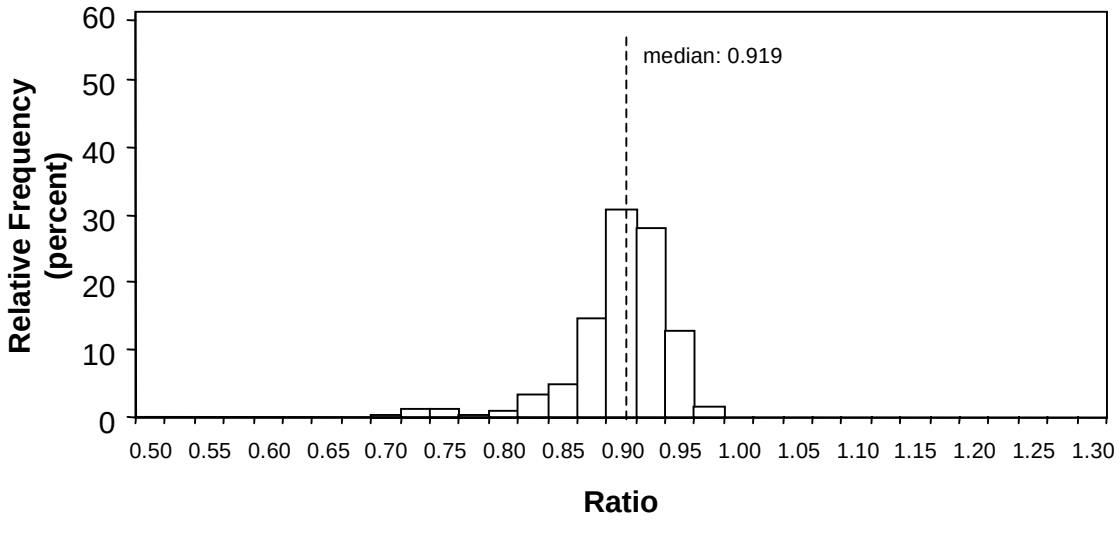


Figure C-26b. Description of Combined RADM/RPM- and REMSAD-Derived Monitor-Level Ratios for Annual Average $PM_{2.5}$ Concentration: 2010 Post-CAAA / 2010 Pre-CAAA



Estimating the Effects of the CAAA on Visibility

Light traveling through the atmosphere is "absorbed" and "scattered" by gases and suspended particles. These distortion processes contribute to total atmospheric light extinction which, in turn, causes visibility degradation. To characterize and ultimately quantify the effect of changes in emissions on visibility, an understanding of the concentrations and types of gaseous particulate constituents in the air is necessary.

The influence of gaseous absorption on light extinction is almost negligible. Gaseous scattering has a larger impact, although this impact is generally not as significant as either particulate absorption or scattering. Together the influence of all four of these light distortion processes is expressed quantitatively as the light extinction coefficient, b_{ext}. In this analysis RADM/RPM and REMSAD are both used to calculate b_{ext}.

RADM/RPM and Visibility

RADM/RPM estimates b_{ext} in the eastern U.S., for each emissions scenario (1990 base year, 2000 Pre-CAAA, 2000 Post-CAAA, 2010 Pre-CAAA, and 2010 Post-CAAA), by combining the influences of particle scattering and absorption and incorporating the effect of scattering caused by water. The fine particles estimated by RADM/RPM (including their associated water) are secondary particulates: sulfates, nitrates, associated ammonium, and organics. Absorption by carbon particles is not included in the model's calculations, nor is extinction resulting from primary particles. By not including these latter influences, RADM/RPM may underestimate the effects of air pollution on visibility.

RADM/RPM, along with generating atmospheric light extinction values, calculates "visual range" and deciview (dV), both measures that quantify visibility. The former, VR, is related to the light extinction coefficient by the following equation:

$$VR(\text{meters}) = 3.912/b_{ext},$$

where b_{ext} is in inverse meters. The latter measure of visibility, dV, and the related DeciView Haze Index are improved indicators of the clarity of the atmosphere. This index more accurately captures the relationship between air pollution and human's perception of visibility than does VR or b_{ext} (Pitchford and Malm, 1994). A deciview is defined by the equation:

$$dV = 10\ln(b_{ext}/10),$$

where b_{ext} is expressed in inverse megameters.

The DeciView Haze Index has a value of approximately zero when the light extinction coefficient is equal to the scattering coefficient for particle-free air. A roughly 10 percent increase in b_{ext} translates to a one unit change in dV. Since the apparent change in visibility is related to a percent change in b_{ext}, equal changes in dV correspond to approximately equally perceptible changes in visibility. Research indicates that, for most observers, a "just noticeable change" in visibility corresponds to an increase or decrease of about one to two dV units. An increase in the deciview level translates to degradation of visibility, while a decrease represents and improvement.

RADM/RPM Modeling Results

For this analysis, under the 1990 base year and future year emissions scenarios, the annual mean daylight hour b_{ext}, VR, and dV were estimated for each RADM/RPM grid cell. A summary of 1990 and 2010 deciview levels for selected cities, metropolitan areas, and national parks is provided in Table C-13. These deciview estimates show that under the Pre-CAAA scenario visibility degradation is expected throughout much of the eastern U.S. Comparison of 1990 base year and 2010 Post-CAAA estimates, however, indicates that with the implementation of CAAA related measures, a perceptible improvement in visibility can be expected.

Table C-13
Comparison of Visibility in Selected Eastern Cities, Metropolitan Areas, and National Parks

		Mean Annual Deciview		
Area Name	**State**	**1990 Base Year**	**2010 Pre-CAAA**	**2010 Post-CAAA**
Acadia NP	ME	11.1	12.0	10.4
Atlanta Metro Area	GA	20.9	22.8	20.0
Boston Metro Area	MA	13.2	14.0	11.9
Chicago Metro Area	IL	17.5	19.1	17.0
Columbus	OH	16.5	17.7	15.1
Detroit Metro Area	MI	16.0	18.5	15.3
Everglades NP	FL	7.6	9.2	6.9
Great Smoky Mtns. NP	TN	20.4	22.3	19.6
Indianapolis	IN	20.1	21.1	19.0
Little Rock	AR	15.0	17.2	15.1
Milwaukee Metro Area	WI	15.6	18.4	15.3
Minn.-St. Paul Metro Area	MN	10.1	12.4	10.3
Nashville	TN	20.4	21.5	19.0
New York City Metro Area	NY/NJ	15.2	18.0	13.9
Pittsburgh Metro Area	PA	15.8	16.9	14.2
St. Louis Metro Area	MO	16.5	17.8	16.0
Shenandoah NP	VA	16.5	17.8	15.2
Syracuse	NY	12.4	13.2	11.5
Washington, DC Metro Area	DC/VA/MD	17.5	19.2	16.3

*For cities, metro areas, or national parks not contained by a single RADM/RPM grid cell, the visibility measure presented in this table is a weighted average of the mean annual deciview level from each of the grid cells that together completely contain the selected area. Weighting is based upon the spatial distribution of an area over the various grid cells.

REMSAD and Visibility

REMSAD was used to estimate the effect of changes in emissions on visibility for the western U.S. This model calculates light extinction coefficients based upon estimates of the gridded ground-level concentrations of the following species – sulfate (NH4S+GSO4+ASO4), nitrate (NH4N+PNO3), NO2, SOA, POA, PEC, PMfine and PMcoarse (refer to Table C-8 for a description of these species abbreviations). The contribution from each of these species is adjusted based on the extinction efficiency of each and, in the case of sulfate, nitrate and SOA, an adjustment dependent on the relative humidity. The total extinction coefficient is then given by:

b_{ext} = 10.+ 0.17*NO2 + f_{so4}(RH)*sulfate + f_{no3}(RH)*Nitrate + f_{soa}(RH)*SOA +6.2*POA + 10.5*PEC + PMFINE + 0.6*PMCOARSE

where the constant value of 10.0 is the contribution to the scattering coefficient for particle-free air (Rayleigh scattering). REMSAD generated b_{ext} values are then converted to deciviews.

REMSAD Modeling Results

Visibility estimates and change in visibility were calculated for each of the future-year scenarios for use in the effects analysis. Figure C-27 illustrates 1990 base year deciview levels for the western U.S. This map shows that visibility is poorer in the region of California extending from San Francisco southward to Los Angeles, the Pacific Northwest, and larger metropolitan areas such as Denver, CO; Albuquerque, NM; and Phoenix, AZ. Most noticeable is the comparatively high deciview level in the Los Angeles region.

Figures C-28 and C-29 illustrate the difference between 2010 Pre-CAAA and 1990 base year estimates and the difference between 2010 Post-CAAA and 1990 base year estimates, respectively. The first of these maps shows that under the Pre-CAAA scenario visibility is expected to remain unchanged between 1990 and 2010 throughout much of the West and actually improve in coastal Oregon and along the western Idaho border. In the larger urban areas, however, perceptible visibility degradation is predicted. Visibility improvement in and around western cities, especially in California, is predicted under the Post-CAAA scenario. Figure C-29 captures these changes and shows that in 2010 improvements in visibility are not expected to be restricted to just the larger urban areas; compared to 1990 base year estimates, Post-CAAA deciview levels are also predicted to be lower throughout much of Washington, Oregon, and Nevada and in sizeable sections of Arizona, Idaho, Utah, and Wyoming.

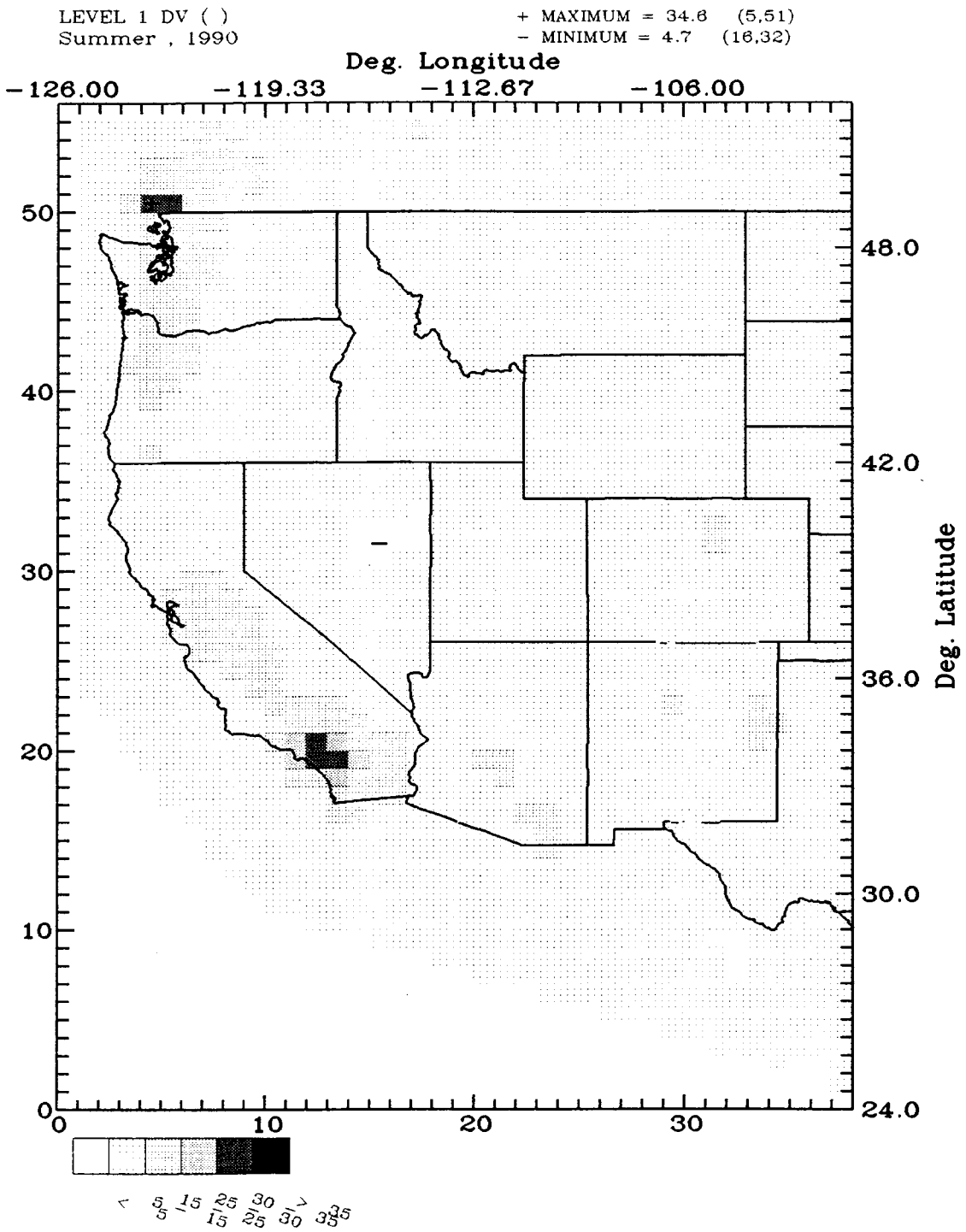


Figure C-27. Seasonal Average Deciview for the summer REMSAD simulation period (1-10 July 1990): base 1990 (western U.S. only)

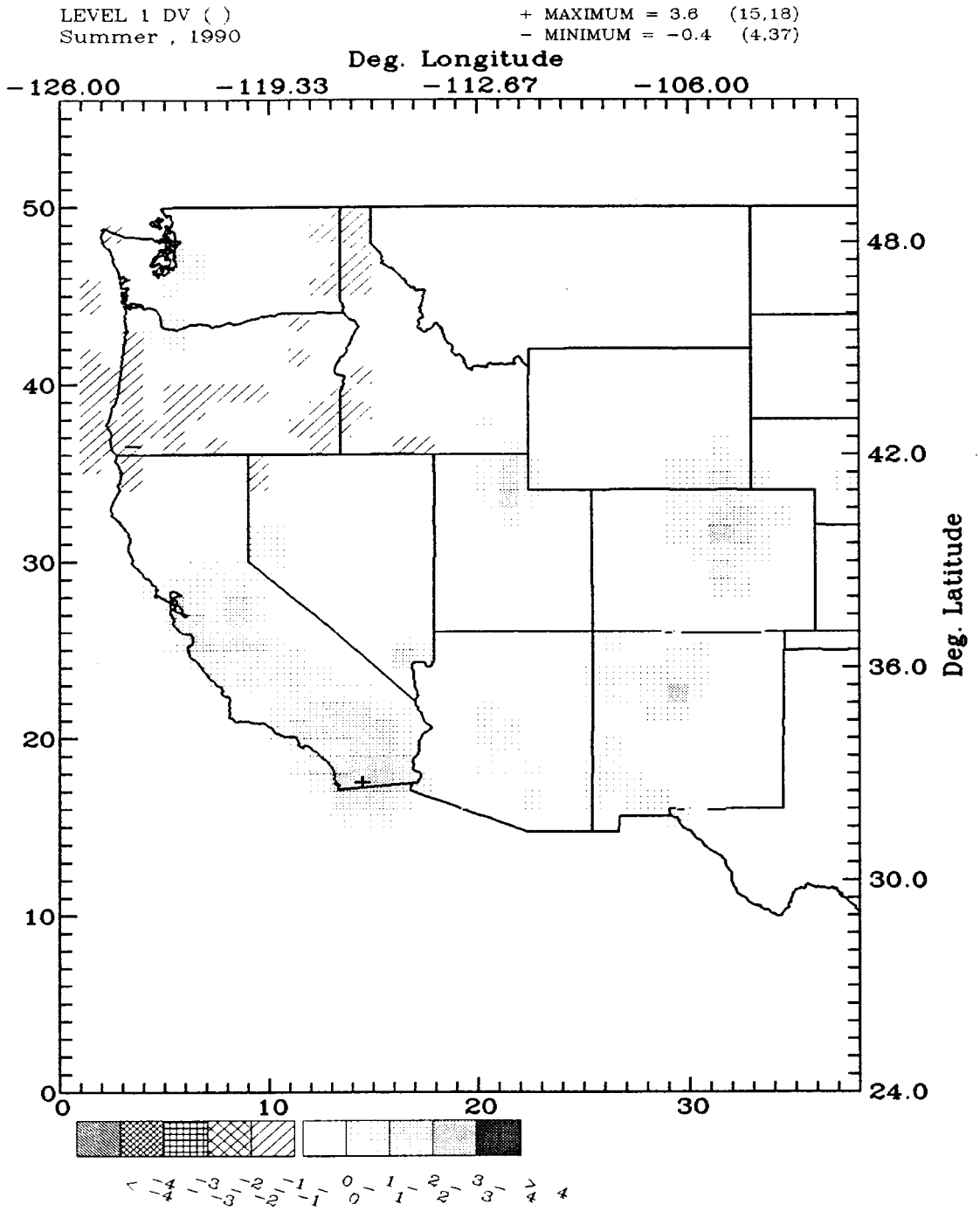


Figure C-28. Difference in seasonal average Deciview for the summer REMSAD simulation period (1-10 July 1990): 2010 pre-CAAA90 minus base 1990 (western United States only)

Acid Deposition

The acid deposition modeling efforts for this analysis focused on estimating the change in ambient concentrations of selected pollutants as a result of changes in emissions. The need to focus on relative changes, rather than absolute predictions, is especially acute when estimating air quality outcomes for pollutants subject to long-range transport, chemical transformation, and atmospheric deposition. The complexity of the relationships between emissions, air concentrations, and deposition is well-described in the following paragraph from the RADM report document developed by Robin Dennis of U.S. EPA's National Exposure Research Laboratory:

> *"Sulfur, nitrogen, and oxidant species in the atmosphere can be transported hundreds to thousands of kilometers by meteorological forces. During transport the primary emissions, SO_2, NO_x, and volatile organic compounds (VOC) are oxidized in the air or in cloud-water to form new, secondary compounds, which are acidic, particularly sulfate and nitric acid, or which add to or subtract from the ambient levels of oxidants, such as ozone. The oxidizers, such as the hydroxyl radical, hydrogen peroxide and ozone are produced by reactions of VOC and NO_x. The sulfur and nitrogen pollutants are deposited to the earth through either wet or dry deposition creating a load of pollutants to the earth's surface... However, the atmosphere is partly cleansed of oxidants through a number of physical processes including deposition (e.g., ozone is removed by wet and dry deposition). Dry deposition occurs when particles settle out of the air onto the earth or when gaseous or fine particle species directly impact land, plants, or water or when plant stomata take up gaseous species, such as SO_2. In wet deposition, pollutants are removed from the atmosphere by either rain or snow. In addition, fine particles or secondary aerosols formed by the gas- and aqueous-phase transformation processes scatter or absorb visible light and thus contribute to impairment of visibility."*[10]

[10] Dennis, R. RADM Report (1995), p. 1.

The complexity and nonlinearity of the relationships between localized emissions of precursors, such as SO_2 and VOCs, and subsequent regional scale air quality and deposition effects are so substantial that advanced modeling is required to accurately estimate the broad-scale impact of changes in emissions on acid deposition. For this analysis, EPA used the Regional Acid Deposition Model (RADM) to estimate acid deposition in the eastern United States.

Overview of the RADM Modeling System

RADM, a three-dimensional Eulerian grid-based model also used in the PM analysis, estimated nitrogen and sulfur deposition for the 1990 base year and each of the future year emissions scenarios. Estimates, expressed in kg/ha, were developed for 2000 and 2010 and calculated for each 80-km RADM grid cell. It is important to note, however, that ammonia deposition, a significant contributor to total nitrogen deposition, was held constant for each of the model runs. This was because livestock farming and other activities that drive ammonia formation and deposition were essentially unaffected by the CAAA-related control programs. A more detailed description of RADM, its domain, and its inputs is provided earlier in this appendix..

RADM Modeling Results

Figures C-30 and C-31 show the 1990 base-year deposition estimates for sulfur and nitrogen respectively. Predictions for both pollutants under the Pre- and Post-CAAA scenarios are displayed in Figures C-32 through C-35. Comparison of the three maps showing sulfur deposition and comparison of the three maps showing nitrogen deposition reveals that for both pollutants annual deposition under the Pre-CAAA scenario is expected to increase between 1990 and 2010. Year 2010 Post-CAAA sulfur and nitrogen deposition projections, however, are not only lower than 2010 Pre-CAAA projections, but also below 1990 base year levels. Together, these maps indicate that between 1990 and 2010 average annual

acid deposition is expected to decrease as a result of the Clean Air Act Amendments.

Noticeable in each of the figures, especially those mapping nitrogen, is an area of high deposition along the Virginia-North Carolina border. This "hot spot" is above Person County, NC, a region with one large and one very large utility plant.[11] Emissions from these plants, particularly NO_x, likely are the source of the high deposition in this area. Person County exhibits the highest base year and future year Pre- and Post-CAAA acid deposition estimates in the entire RADM domain.

Comparison of 2010 Pre- and Post-CAAA emissions in Person County shows that NO_x emissions are expected to be lower in 2010 as a result of the CAAA. This change in emissions, however, translates to a change in acid deposition that is not captured by the maps provided in this section. 2010 Post-CAAA nitrogen and sulfur deposition estimates for this county are 27.2 and 78.0 kg/ha respectively. These figures represent a decrease in nitrogen deposition of 14.0 kg/ha and a decrease in sulfur deposition of 4.5 kg/ha from 2010 Pre-CAAA levels. Compared to the base year, the 2010 Post-CAAA nitrogen deposition estimate for Person County is 4.1 kg/ha lower than 1990 levels, the 2010 Post-CAAA sulfur deposition prediction, however, is 12.9 kg/ha higher.

[11]Under the 2010 Post-CAAA scenario the Mayo (large) and Roxboro (very large) utility plants are predicted to emit 9,400 and 30,100 tons of NO_x per year respectively.

Figure C-29
Annual Sulfur Deposition
1990 Base Case Scenario

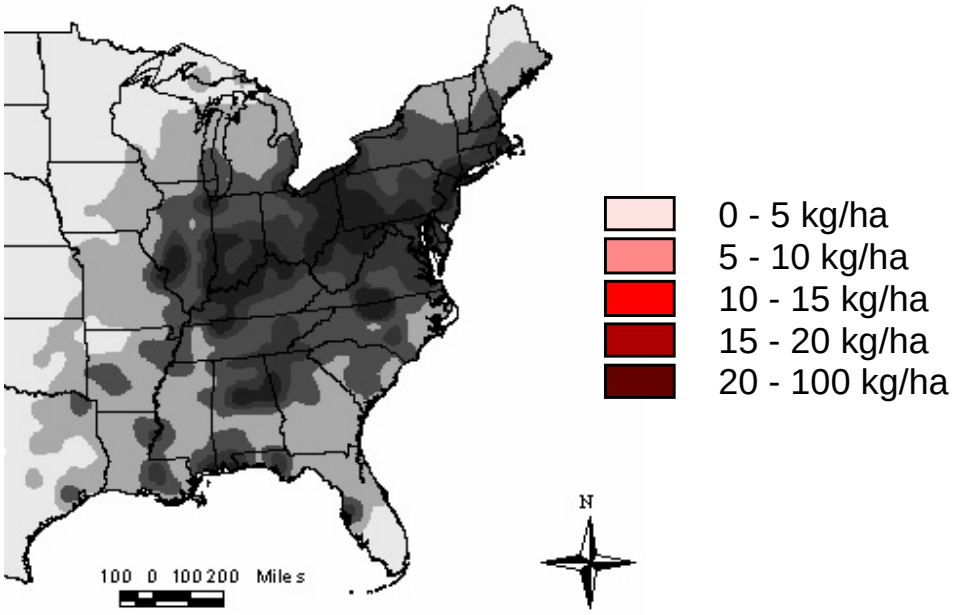


Figure C-30
Annual Nitrogen Deposition
1990 Base Case Scenario

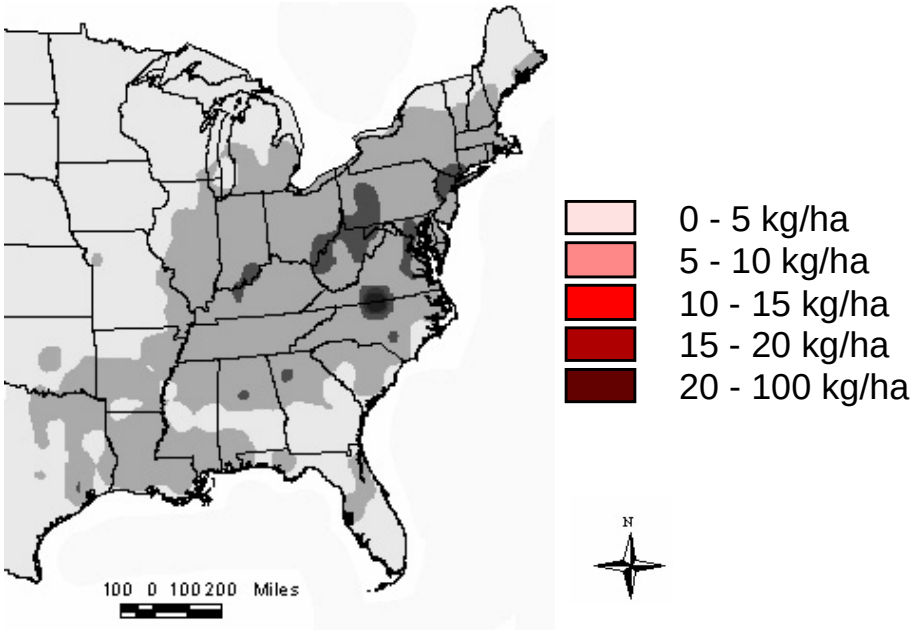


Figure C-31
Annual Nitrogen Deposition
2000 Pre CAAA Scenario

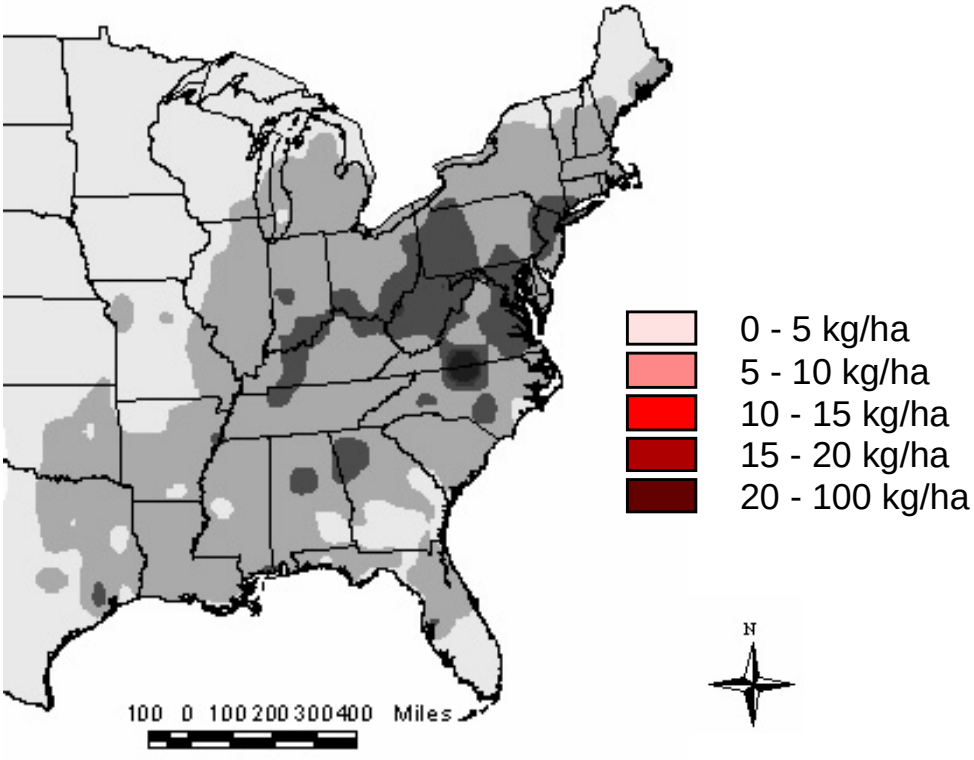


Figure C-32
Annual Sulfur Deposition
2010 Post CAAA Scenario

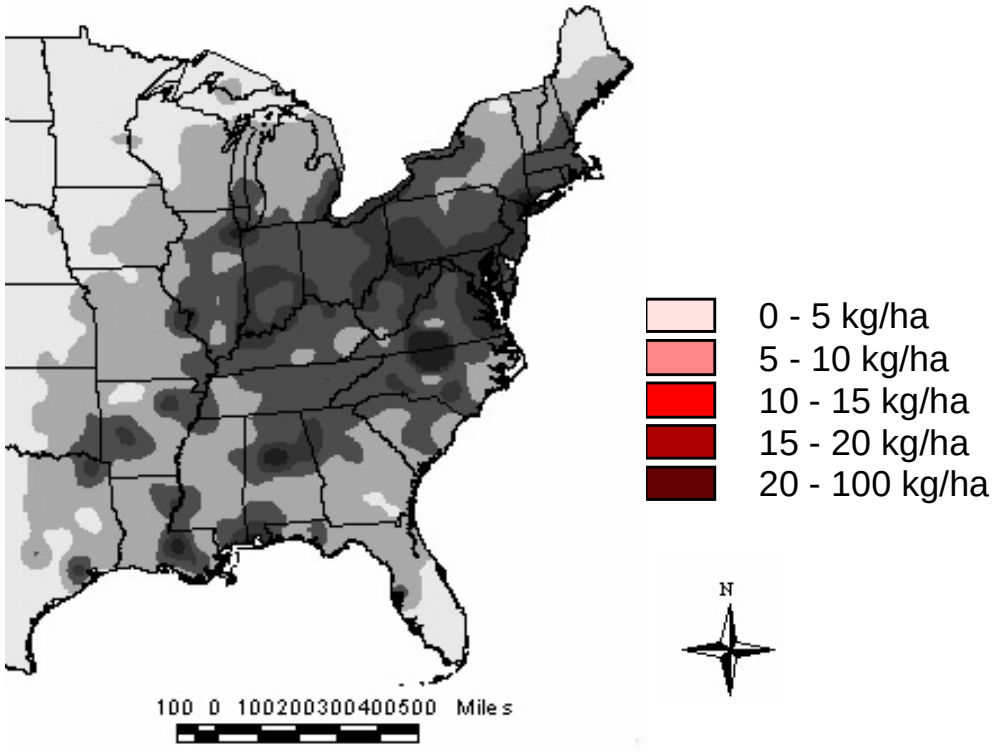


Figure C-33
Annual Nitrogen Deposition
2010 Pre CAAA Scenario

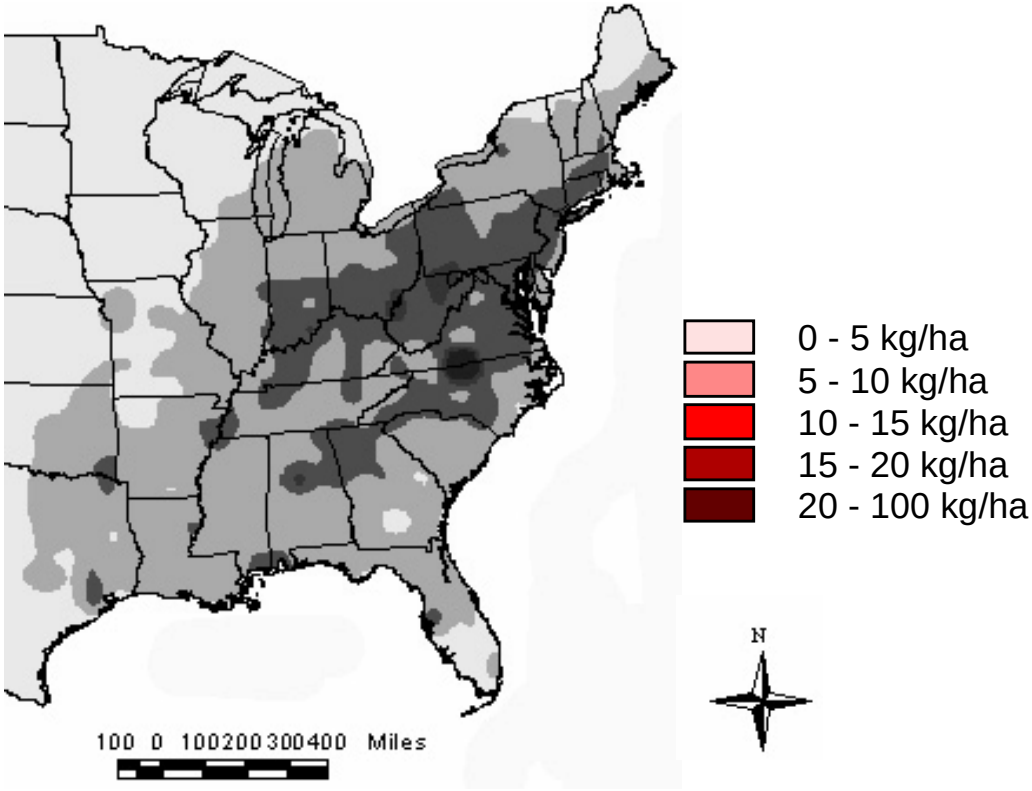
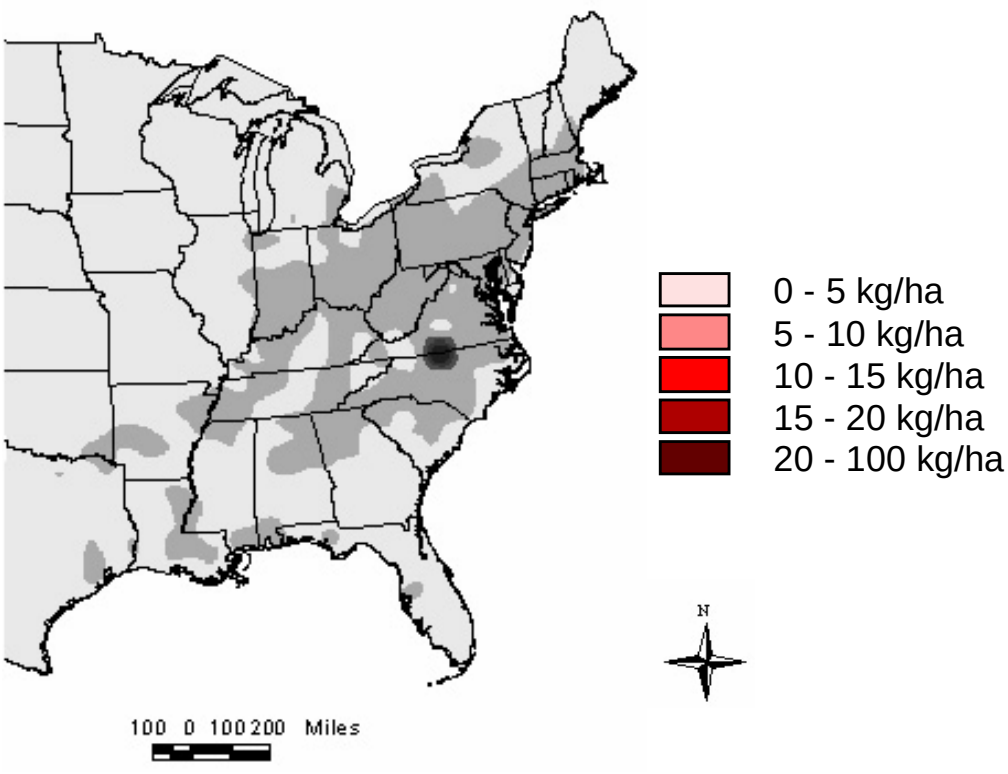


Figure C-34
Annual Nitrogen Deposition
2010 Post CAAA Scenario



Estimating the Effects of the CAAA on Sulfur Dioxide, Oxides of Nitrogen, and Carbon Monoxide

Future-year Pre- and Post-CAAA ambient SO_2, NO, NO_2, and CO concentrations were estimated by adjusting 1990 concentrations using future-year to base-year emissions ratios. The methodology for calculating and applying these ratios is described below. The resulting future-year concentration also are discussed in this section; histograms are used to illustrate the relationship between Post- and Pre-CAAA emissions estimates.

Methodology for Estimating Future-Year SO_2, NO, NO_2, and CO Concentrations

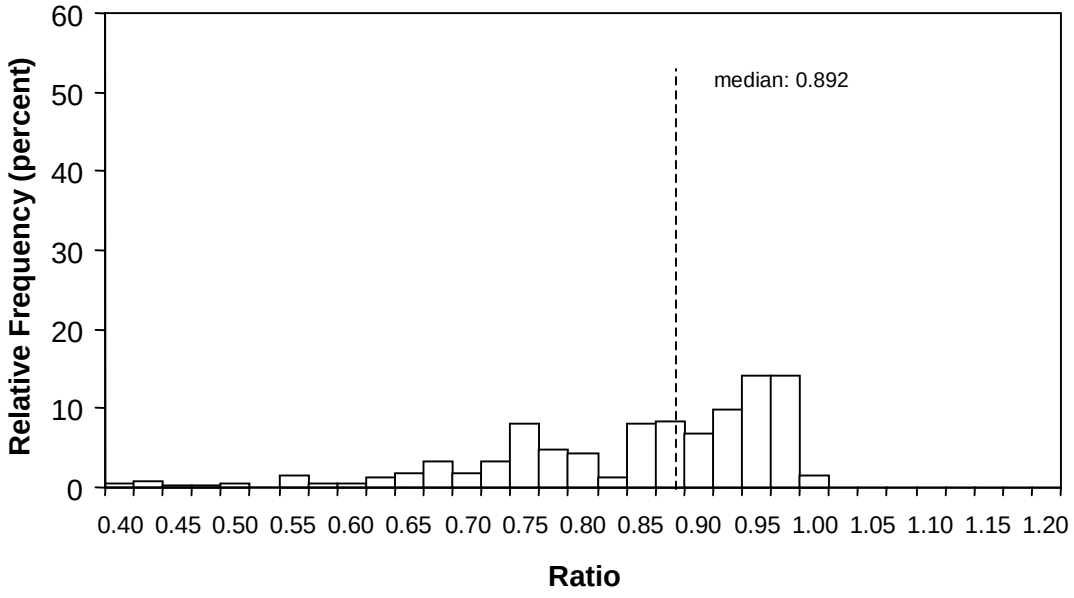
To estimate future-year SO_2, NO, NO_2, and CO concentrations, adjustment factors were calculated using grid cell specific REMSAD emissions data (Douglas et al., 1999). REMSAD's domain encompasses the 48 contiguous states and is divided into 4,950 grid cells, each measuring approximately 56 km by 56 km. As part of the model's input, gridded emission inventories containing seasonal Pre- and Post-CAAA SO_2, NO, NO_2, and CO emissions estimates were prepared. These same emissions estimates used as REMSAD input in other parts of this prospective analysis, were also used to calculate SO_2, NO, NO_2, and CO adjustment factors.

Before emission-based ratios (adjustment factors) were calculated, two separate inventories maintained individually for REMSAD modeling purposes, one containing elevated point source emissions data and the other containing emissions data for low-level sources, were combined. Each stack corresponding to an elevated point source was assigned to a grid cell based on location. Emissions from elevated point sources were then added to the low-level emissions corresponding to the grid cell in which the stack is located. In this manner, a file containing total emissions for each grid cell was prepared. This was done for each season for the 1990 base year and 2000 and 2010 Pre- and Post-CAAA scenarios.

Once the emissions inventory was prepared, emission-based ratios for SO_2, NO, NO_2, and CO were generated. For each RADM grid cell, adjustment factors were calculated comparing future-year (2000 and 2010) emissions under each projection scenarios to base-year (1990) emissions. Separate sets of ratios were developed for each season.

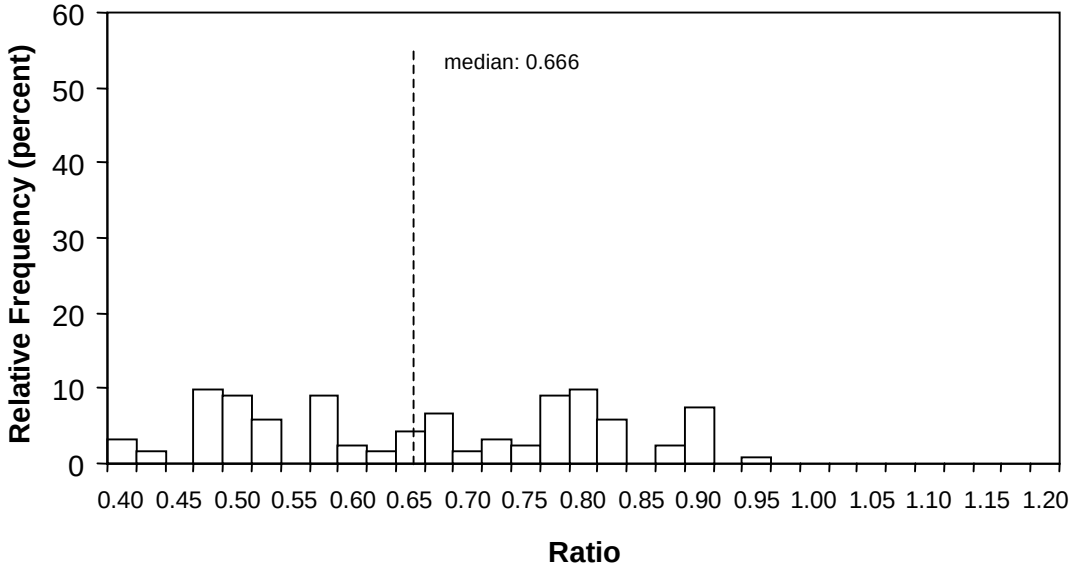
Following the calculation of emission-based ratios, future-year concentrations were then estimated by applying these ratios to observed 1990 base-year monitor concentrations. For REMSAD grid cells without 1990 monitor concentration data interpolation was used to estimate base-year concentrations. Adjustment factors for the grid cell were then applied to the interpolated values.

Figure C-35. Distribution of Monitor-Level Ratios of Summer SO_2 Emissions: 2010 Post-CAAA / 2010 Pre-CAAA



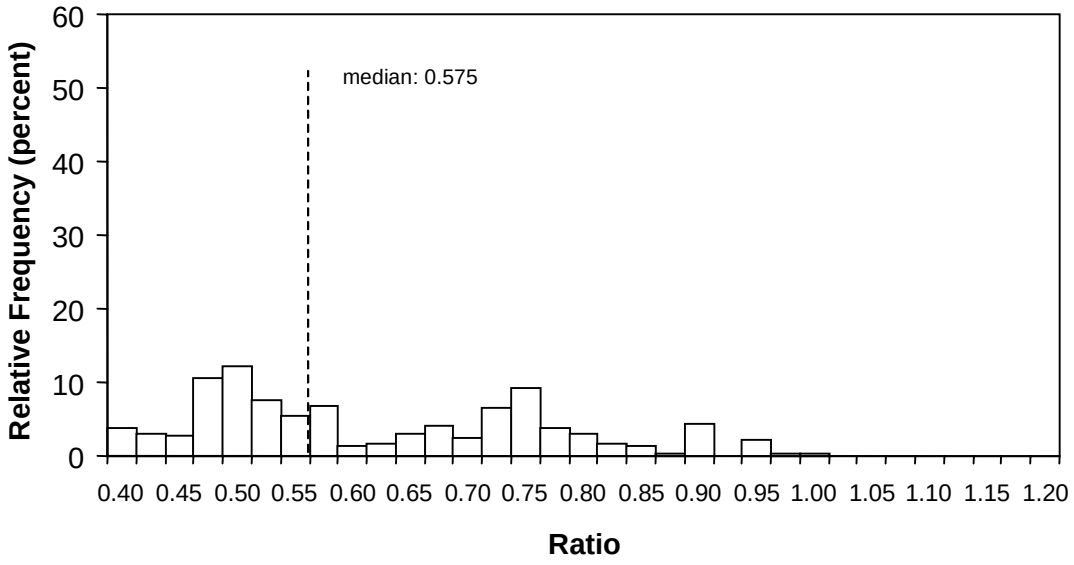
Note: 2.4 percent of the distribution of ratios is less than 0.40.

Figure C-36. Distribution of Monitor-Level Ratios of Summer NO Emissions: 2010 Post-CAAA / 2010 Pre-CAAA



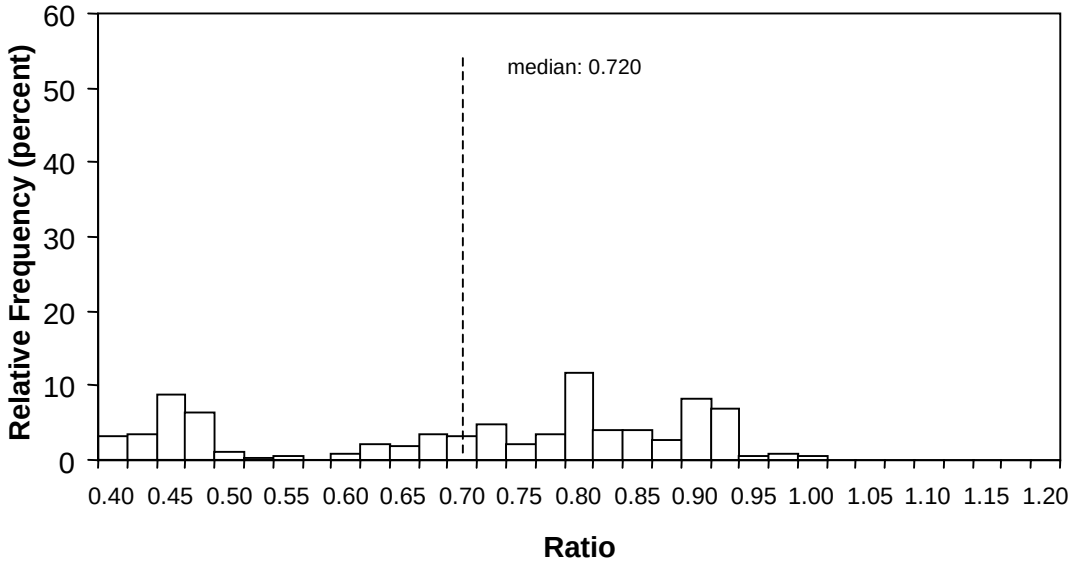
Note: 3.3 percent of the distribution of ratios is less than 0.40.

Figure C-37. Distribution of Monitor-Level Ratios of Summer NO_2 Emissions: 2010 Post-CAAA / 2010 Pre-CAAA



Note: 2.7 percent of the distribution of ratios is less than 0.40.

Figure C-38. Distribution of Monitor-Level Ratios of Summer CO Emissions: 2010 Post-CAAA / 2010 Pre-CAAA



Note: 15.7 percent of the distribution of ratios is less than 0.40.

Emission-Based Ratios for SO_2, NO, NO_2, and CO

Emission-based ratios were calculated for each grid cell, regardless of whether or not the cell contained a monitoring site. The figures included in this section however, represent the distribution of ratios for actual monitoring site locations. These distributions reveal the relationship between future-year and base-year concentrations. A ratios greater that one indicates an increase in ambient concentration from the base-year, while a ratio less than one indicates a decrease.

Our results indicate that compared to the base-year, future-year concentrations of SO_2, NO, NO_2, and CO tend to increase under the Pre-CAAA scenario, while Post-CAAA concentrations for all four pollutants except SO_2 tend to decrease. For example, the median 2010 Pre-CAAA emission-based ratio for SO_2 is roughly 1.35, indicating an increase in median 2010 Pre-CAAA SO_2 concentration of approximately 35 percent from the 1990 base-year. The median ratios for NO, NO_2, and CO are roughly 1.13, 1.17, and 1.05 respectively. Under the Post-CAAA scenario we estimate that in 2010 NO, NO_2, and CO concentrations will tend to be approximately 25 and 30 percent below base-year levels. The median 2010 Post-CAAA emission-based ratios for these three pollutants are roughly 0.74, 0.70, and 0.76 respectively. We estimate that SO_2, concentrations, however, will increase in many areas of the U.S. The median adjustment ratio for this pollutant is approximately 1.21.

Comparison of the Pre- and Post-CAAA Ratios

Comparison of Pre- and Post-CAAA emission-based adjustment factors also helps illustrate the effect of the 1990 Amendments on ambient pollution concentrations. The ratio of 2010 Post-CAAA adjustment factors to 2010 Pre-CAAA adjustment factors shows the impact of the 1990 Amendments on ambient concentrations relative to the baseline scenario. Ratios less than one indicate that we estimate that future-year concentrations of SO_2, NO, NO_2, and CO are lower under the Post-CAAA scenario than under the Pre-CAAA scenario.

Figures C-35 through C-38 show the distribution of 2010 Post-CAAA to 2010 Pre-CAAA ratios for summertime SO_2, NO, NO_2, and CO respectively. These figures illustrate the regional variation in the influence of the 1990 Amendments on ambient concentrations of these pollutants. Although we estimate concentrations in some areas will increase under the Post-CAAA scenario relative to Pre-CAAA estimates, the median summertime 2010 Post- to Pre-CAAA ratios for SO_2, NO, NO_2, and CO are 0.90, 0.67, 0.58, and 0.72 respectively. These values, each less than one, indicate that the central tendency for summertime 2010 Post-CAAA concentration estimates of these four pollutants is to be lower than 2010 Pre-CAAA estimates.

Table C-14 displays the median values of the distribution of Post- to Pre-CAAA ratios for the summer months described above and the remaining three seasons. Just as for the summer; spring, autumn, and winter median values are less than one. Averaged over all four seasons, we estimate a median reduction in SO_2, NO, NO_2, and CO concentrations of approximately 9, 33, 40, and 25 percent respectively. RACT requirements, tailpipe emissions standards, and NO_x emissions trading account for the bulk of the reduction in NO and NO_2 concentrations. Title I nonattainment area controls and Title II motor vehicle provisions are responsible for much of the change in CO concentrations, while regulation of utility and motor vehicle emissions account for majority of the decrease in SO_2 concentrations.

Table C-14
Median Values of the Distribution of Ratios of 2010 Post-CAAA/Pre-CAAA Adjustment Factors

	SO_2	NO	NO_2	CO
Spring	0.904	0.669	0.598	0.790
Summer	0.892	0.666	0.575	0.720
Autumn	0.916	0.677	0.614	0.756
Winter	0.924	0.686	0.626	0.692

Table C-15
Background Concentrations used to Prepare the SO_2, NO, NO_2, and CO Profiles

Pollutant	Background Concentration
SO_2	0
NO	0
NO_2	0
CO	0.2 ppm

Attributes and Limitations of the Modeling Analysis Methodology

The Section 812 prospective modeling analysis utilized a set of modeling tools and input databases that for the most part had been developed, tested, and evaluated as part other modeling studies (e.g., OTAG, SIP modeling analyses, etc.). This provided a cost-effective means of conducting a national-scale modeling exercise. The models used for the study are among the most widely used and evaluated tools for ozone and PM modeling, and have been used for previous regulatory applications. The modeling was performed in manner that is consistent with established practice and EPA guidelines regarding air quality model applications.

Although appropriate techniques were used for the analysis of each pollutant, use of separate models/techniques for the analysis of ozone, PM, and the other criteria pollutants does not allow a fully integrated analysis of the effects of each. Consequently, the results do not reflect all potential interactions between pollutants (e.g., ozone and PM). Ongoing research involving the development and testing of integrated modeling tools (by EPA and other organizations) may provide the opportunity for fully integrated future Section 812 prospective modeling efforts.

Analysis of the effects on the national scale (the CAAA applies to the entire nation) required the use of several different domains with varying grid resolution as well as the use of relatively coarse resolution for many areas of the country for the grid-based modeling effort. The use of relatively coarse grid resolution (12 km and greater) is a potentially important source of uncertainty with respect to the modeling results. Previous studies have found that the response of the UAM-V modeling system to emission reductions is affected by grid resolution (Douglas et al., 1996). Thus, the use of grid-cell specific adjustment factors to modify site-specific data may introduce some uncertainty into the future-year estimates.

There are always uncertainties associated with the use of modeling results to estimate future-year air quality. These derive from inaccuracies in the model inputs and/or model formulation and were manifested in this study in the evaluation of model performance. While good model performance was

achieved for most model applications, ozone concentrations were underestimated within the Los Angeles domain and PM concentrations were underestimated during the fall and winter simulation periods in the REMSAD application. RADM/RPM, used as part of the PM and visibility analyses, showed a tendency to overestimate annual average sulfate concentrations and warm season nitrate concentrations. Annual average nitrate predictions generated by RADM/RPM, however, matched air quality monitor data.

The acid deposition estimates included in the present analysis are limited to the eastern states within the RADM domain. Deposition in the western U.S. was not modeled for this study. Although acid deposition is a problem primarily for the eastern U.S., deposition does occur in states west of the RADM domain. The magnitude of the benefits of reducing acid deposition in these western states is likely to be small, however, relative to the overall benefits associated with the Clean Air Act Amendments.

The approach used in this study to estimate future air quality (the combined use of observed data and modeling results) may, compared to a more standard air quality model application (e.g., a model application for attainment demonstration purposes), tend to minimize the effects of many of the uncertainties mentioned in this section. The reason for this is that the modeling results are used in a relative sense, rather than an absolute sense. This may enhance the reliability of the future-year concentration estimates, especially in the event that the uncertainty inherent in the absolute concentration values is greater than that associated with the response of the modeling system to changes in emissions.

The ratios for adjusting the observed data are calculated using modeling results for a limited number of simulation days and it is assumed, using this methodology, that the ratios can be used to represent longer time periods. This approach permits the estimation of seasonal and annual concentration distributions. Nevertheless, the use of the model-based ratios in adjusting data for an entire season or year may result in some over- or underestimation of the benefits of the simulated control measures, depending upon whether the simulation results for the modeled days are sufficiently representative of the meteorological and air quality conditions that occurred during 1990.

Finally, there are numerous ways in which the adjustment factors could be calculated and applied. The approach used in this study was designed to make the best use of the information and level of detail present in both the observations and the modeling results (e.g., use of decile and quintile based ratios for ozone and PM, respectively). The specific assumptions employed in the application of the methodology, however, may affect the resulting air quality profiles and should be carefully considered in the subsequent use and interpretation of the results.

Conclusions and Recommendations for Further Research

The results from the air quality modeling component of the Section 812 prospective analysis indicate that for both future years (2000 and 2010), the measures and programs associated with the CAAA are expected to result in lower concentrations of ozone, PM, and the other criteria pollutants compared to a future-year scenario without such programs. The degree of improvement in air quality varies among the criteria pollutants and the various portions of the country included in the modeling analysis. The results also differ between the two future years, such that the improvements are greater and more widespread for 2010.

The modeling analysis relied on a set of modeling tools and input databases that (for the most part) had been developed, tested, and evaluated as part other modeling studies. It also made use of several of the most widely used and comprehensively tested tools for ozone and PM modeling. The modeling was performed in a manner that is consistent with established practice and EPA guidelines regarding air quality model applications. However, as noted in the

previous section of this report, there are several features of the modeling analysis that could be improved upon, especially considering recent advances in the development of integrated modeling tools and techniques. Recommendations for future air quality modeling efforts to support the Section 812 prospective analyses include:

- Selection of modeling episode periods using an integrated episode selection procedure (e.g., Deuel and Douglas, 1998) such that the modeling periods are representative of the historical meteorological and air quality conditions and can be used to represent seasonal and annual ozone, PM, and visibility metrics

- Reconfiguration of the modeling domain(s) such that a consistent use of high-resolution grids over urban areas with complex meteorological or emissions-based features are accommodated.

- Review and update of the input data and input preparation techniques to include, for example, updated (more recent) emissions estimates (anthropogenic and biogenic), higher-resolution meteorological inputs, enhanced estimates of future land-use patterns (reflecting growth of urban areas, changes in the interstate transportation networks, etc.).

- Use of an integrated modeling tool for the simultaneous analysis of the effects of emissions changes on ozone, PM, and other pollutants (several tools, including MODELS-3 and UAM-VPM, are currently undergoing development and testing). A comprehensive evaluation of model performance will be required.

- Continued review and enhancement (as appropriate) of the methodology for the combined use of observed data and modeling results.

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